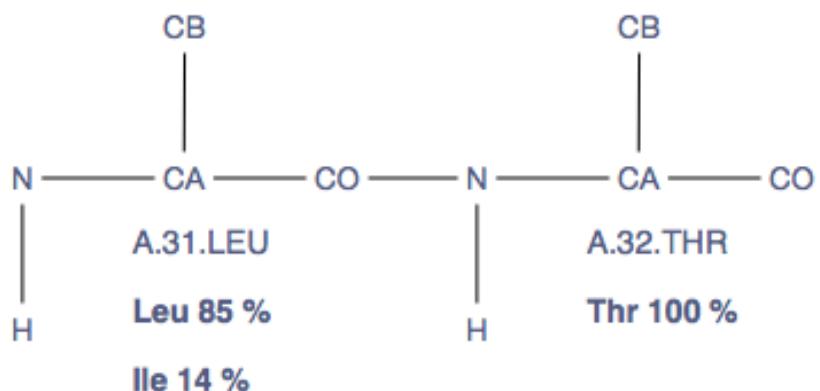
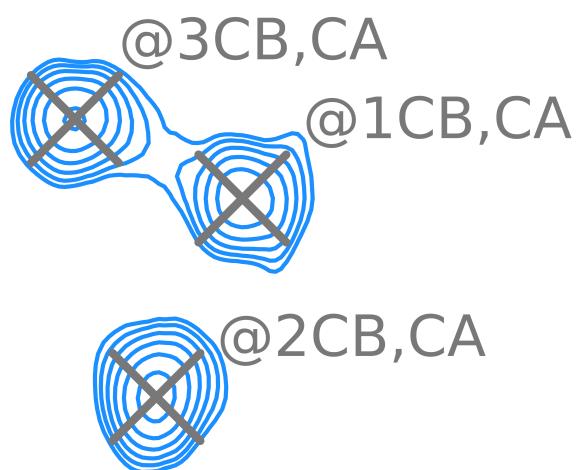


Solid State Assignment Tutorial



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Introduction

This tutorial is designed to introduce you to a variety of tools and features which are useful for the assignment of carbon-detected solid-state protein NMR spectra using CcpNmr AnalysisAssign Version 3.0. It is not intended to teach any theoretical aspects of NMR assignment. For more details about procedures to assign proteins in the solid state see [Higman, VA \(2018\) Progress in NMR Spectroscopy 106–107, 37–65.](#)

It is assumed that you have some basic familiarity with the program, e.g. from having completed our [Beginners Tutorial](#).

In this tutorial you will use spectra recorded on the SH3 domain of chicken alpha-spectrin, in particular PDSD, NCACX and NCOCX spectra recorded on uniformly labelled protein and protein labelled using 1,3-¹³C and 2-¹³C-labelled glycerol. We are grateful to Prof. Hartmut Oschkinat for making these spectra available to us.

You will need to use the project which is located in the directory: AnalysisV3/data/SH3SolidStateTutorial.

Please note that the images shown are only representative and you may encounter minor differences in your setup.

Contents:

1. Project Setup
2. Working with 3D spectra
3. Spin System Identification
4. Making Sequential Links
5. Sequence Specific Assignments
6. Further Assignments
7. Other Useful Tools

Start CcpNmr Analysis V3

Apple users by double clicking the icon
CcpNmrAnalysis



Linux users by using the terminal command: *bin/assign*

Windows users by double-clicking on the *assign.bat* file

Getting started, basic operations

Sidebar

All data contained in a project, such as spectra and peak lists are located in the sidebar. **Double-clicking** on an item will open the properties popup.

Display

A display can contain multiple overlaid spectra which share the same axes.

To show/hide a single spectrum, click on its toolbar button. If you close a display, you can open a spectrum by **dragging and dropping** it into the drop area from the sidebar or **right-clicking** on a sidebar item and selecting **Open as module**. You can also add additional spectra to a spectrum display module later on, or drag several spectra into the drop area together to open them simultaneously.

Mouse

- Pan → **Left-drag** in display
- Zoom in/out → **Scroll wheel** in display
- Context menu → **Right-click**
- Select a peak → **Left-click** on a peak symbol “X”
- Move a peak → select first, then **middle-click and drag**

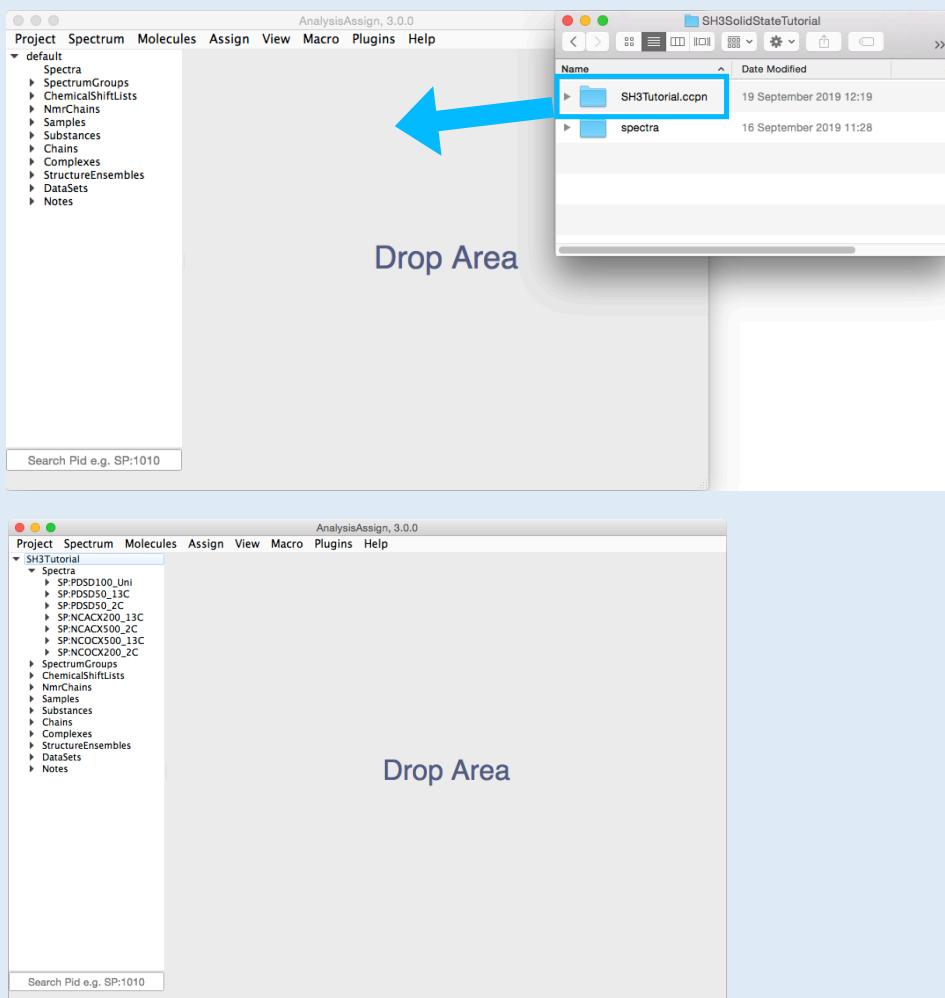
Shortcuts

The program uses several shortcuts, for example **MK** for creating a mark at the current mouse position. You will need to press the first letter on your keyboard e.g. **M**, followed by the second letter, e.g. **K** (case insensitive). Press **Esc** to cancel the first letter.

For more commands and operations:

Main Menu -> *Help* -> *Tutorial (Beginners)* or *Show Shortcuts*

Open the project AnalysisV3/data/SH3SolidStateTutorial/SH3Tutorial ccpn



1A Drag & drop “SH3Tutorial ccpn” into the sidebar or drop area

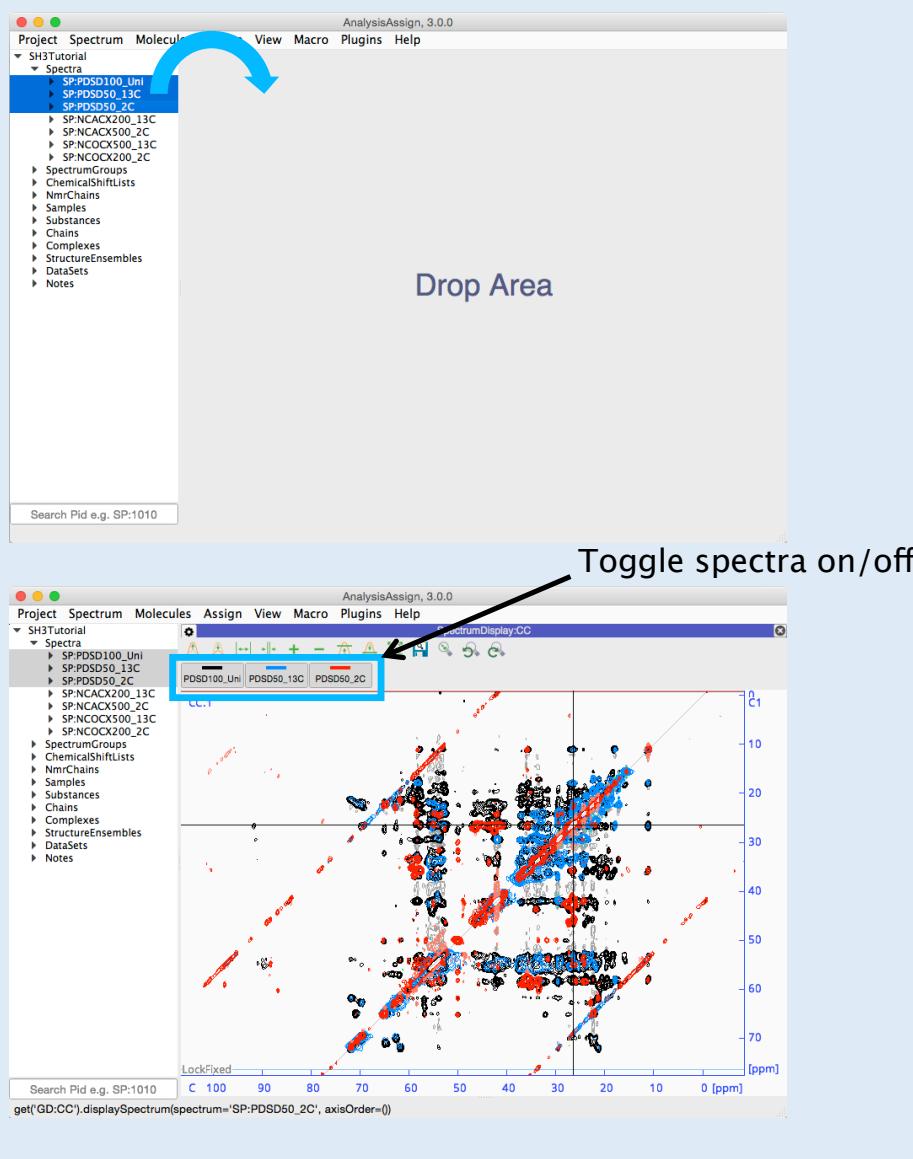
CcpNmr projects have an extension of type “filename ccpn”. Find the project *SH3Tutorial ccpn* in the directory AnalysisV3/data/SH3SolidStateTutorial.

- Select the directory “**SH3Tutorial ccpn**”, drag and drop it into the program.
The SH3 Tutorial project will be loaded.

Nested under **Spectra** in the sidebar, you will have seven spectra. The spectrum names indicate the spectrum type, mixing time and sample labelling:

PDSD100_Uni	PDSD, 100ms mixing time, uniformly labelled sample
PDSD50_13C	PDSD, 50ms mixing time, 1,3- ¹³ C glycerol sample
PDSD50_2C	PDSD, 50ms mixing time, 2- ¹³ C glycerol sample
NCACX200_13C	NCACX, 200ms mixing time, 1,3- ¹³ C glycerol sample
NCACX500_2C	NCACX, 500ms mixing time, 2- ¹³ C glycerol sample
NCOCX500_13C	NCOCX, 500ms mixing time, 1,3- ¹³ C glycerol sample
NCOCX200_2C	NCOCX, 200ms mixing time, 2- ¹³ C glycerol sample

Displaying Spectra



1B Displaying spectra

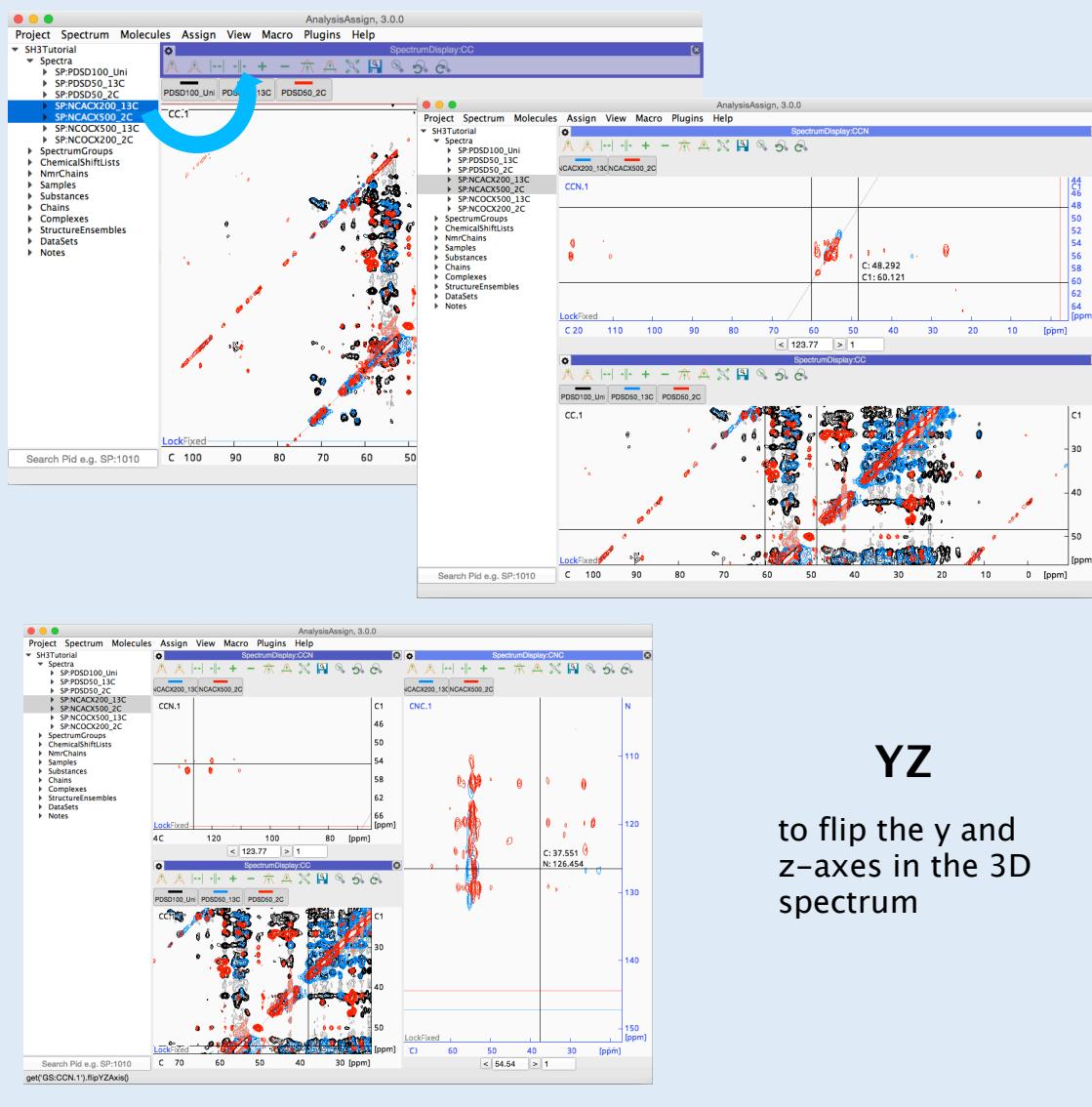
Spectra with the same axes can be shown in the same display. E.g. you can drag all PDSD spectra into the drop area together or drag further spectra into the display once you have opened one of them.

- **Drag** the PDSD spectra into the drop area.
- Use the **Spectrum Buttons** in the toolbar to toggle individual spectra on or off in the display.

The spectra are colour coded according to the isotopic labelling of the samples they were recorded on:

black	uniform ^{13}C , ^{15}N labelling
blue	uniform ^{15}N labelling, 1,3- ^{13}C glycerol labelling
red	uniform ^{15}N labelling, 2- ^{13}C glycerol labelling

Displaying 3D Spectra



2A Displaying the 3D spectra

Your 3D spectra will have to go into a separate display to your PDSD spectra. If at least one spectrum display module is already open, then you can choose where to open a new one. The appearance of a purple box indicates possible drop positions.

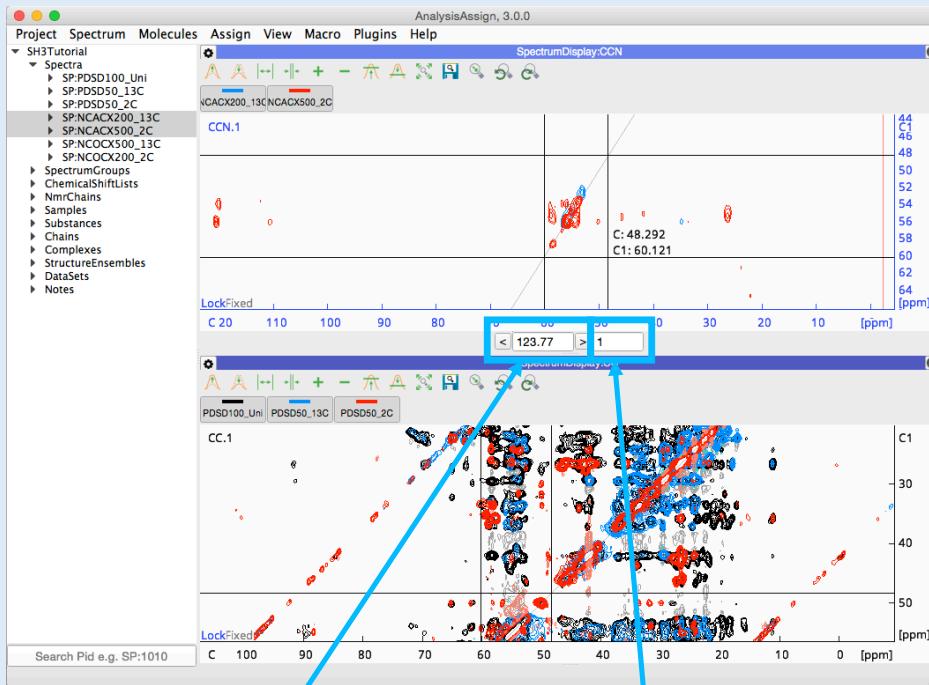
- Drag the NCACX spectra from the sidebar into the drop area.

By default the 3D NCC spectra are shown with ^{15}N on the z-axis. You can easily flip these to show ^{15}N on the y-axis:

- Click on the NCACX spectrum display you want to flip to make sure it is the 'current strip' (its axes are then highlighted)
- Type YZ

This will open a new spectrum display module – close or retain the initial 3D spectrum display module as you wish and re-arrange your modules to suit you.

Navigating through 3D Spectra



use arrows to move through planes, or type a ppm value

change number of visible planes here

2B Navigating through 3D spectra

To move through the z-planes of a 3D spectrum:

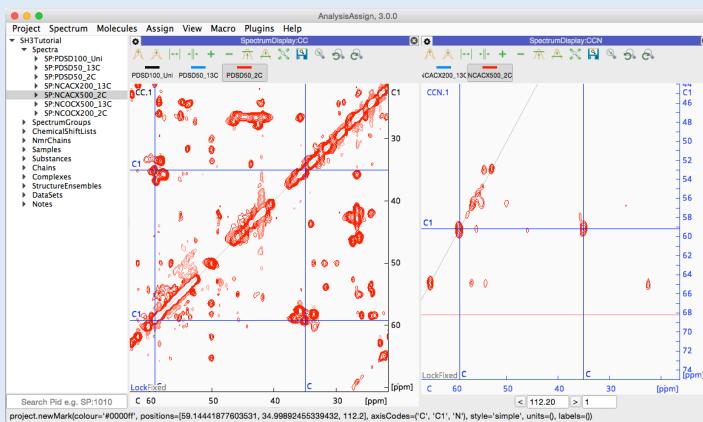
- use the **arrow buttons** either side of the z-position, or
- **type** a ppm value in the box to go to a specific position

Change the number of visible planes by

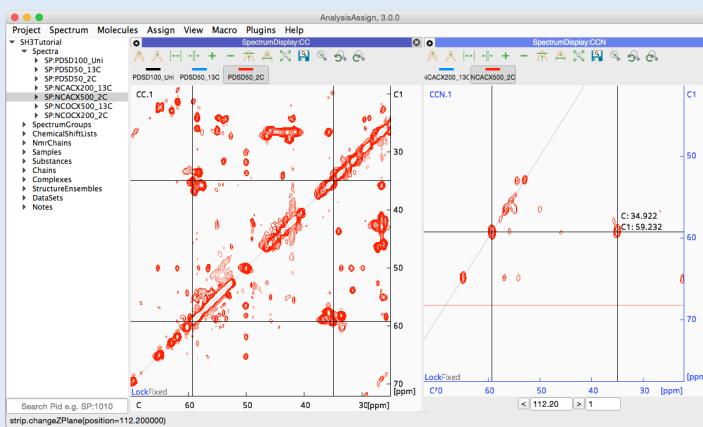
- typing a different number into the planes box

Sometimes it can be useful to move to a neighbouring plane or increase the number of visible planes when trying to pick peaks in 3D spectra.

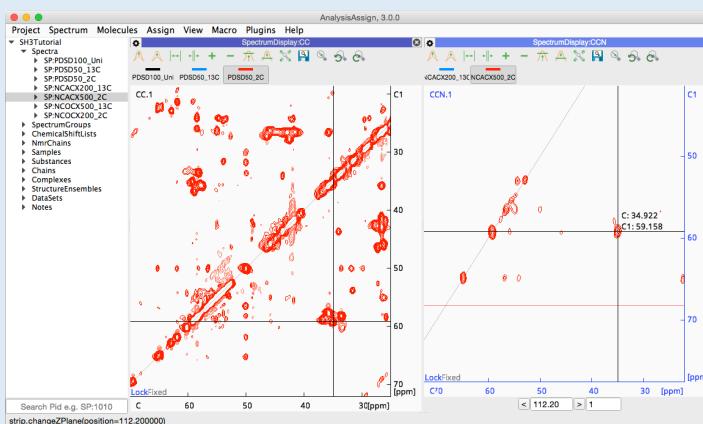
Marks and Mouse Crosshairs



MK Draw mark at mouse position



MC Clear all marks



CD Toggle Double Crosshair on/off

2C Marks and crosshairs

Often it is useful to draw lines through your spectrum to check whether two peaks occur at the same chemical shift or not. A Mark is drawn through all dimensions in all displays at the position where it is placed.

- Place the mouse where you want it to be and type **MK**.
- Clear all your marks by typing **MC**.

It is usually helpful to have the mouse in the double crosshair mode so that all carbon dimensions are linked to one another.

- Toggle this on/off with **CD** or via the **right-hand mouse menu**.

The SH3 domain of chicken α -spectrin contains three threonines. This section will show you how to identify them based on their chemical shifts, pick their peaks, generate NmrAtoms and NmrResidues for them, and assign their atom and amino acid types. Later you will use the 3D spectra and glycerol labelling pattern to sequence specifically assign the threonines.

Assignment nomenclatures (Explanation only)

Assignment in Analysis Assign is simply a matter of setting strings that define the NmrAtoms.

We call this the 'id' (id: identifier) of the NmrAtom. If an id matches the strings defining a molecular Atom¹, this effectively constitutes an assignment to the Atom. If not, the NmrAtom id is a placeholder, reflecting its progress towards assignment².

At this point, it is appropriate also to consider the relationships between Peak, ChemicalShift and NmrAtom. Each dimension of a Peak is assigned to one or more NmrAtoms. The ChemicalShift (which resides in a ChemicalShiftList) of an NmrAtom, is defined by all the peaks that have been assigned to this NmrAtom. Hence, changing an assignment for a Peak (e.g. reassigning a peak from "nmratom_1" to another "nmratom_2") has an effect on the ChemicalShift of "nmratom_1", as it is now no longer defined by the Peak. Likewise, it also affects the ChemicalShift of the "nmratom_2", as it now comes to be (also) defined by the Peak. We will see in next sections how to inspect and change the assignment(s) of a Peak.

If you change the id of an NmrAtom (or its parent NmrResidue or NmrChain), the assignment of all ChemicalShifts and Peaks are updated.

We use NmrChains and NmrResidues to keep track of the NmrAtoms during the assignment process. By default, new NmrResidues are put in NmrChain '@-', and new, temporary NmrChains are given names like '@2'. Initially, NmrChains contain no information about the sequential connections of the NmrResidues, i.e. their ordering. In this case, the NmrChain functions like a simple list with all its NmrResidues.

To store sequential stretches, i.e. lists in which the NmrResidues are ordered, the program uses 'connected' NmrChains, whose names start with '#' instead of '@'. Consequently, names with '@' (and NmrChain names starting with '#') are reserved.

NmrResidues are created with names like '@173' and with no residueType. You can add or change the residueType at any point.

NmrAtom names always start with the nucleus, and default names would be e.g. 'H@31' or 'C@88'. Some names have a special meaning:

- '%' means 'any number', so 'HB%' would be a beta methylene or methyl group. 'H%' would be the backbone NH3 group.
- '*' means 'any string', so 'C*' would be 'any carbon in the residue'
- Names starting with 'M' and 'Q' are (proton) pseudoatom names
- Number suffixes follow NEF (IUPAC) convention, so serine HB2 or HB3 denote stereospecific assignments.
- Suffixes 'x' and 'y' are used for non-stereospecific pairs – the normal assignment to serine beta would use HBx and HBy. For e.g. isopropyl groups the x and y assignments match up between ^1H and ^{13}C so that Leu HDx% are the methyl protons bound to Leu CDx (NEF convention).

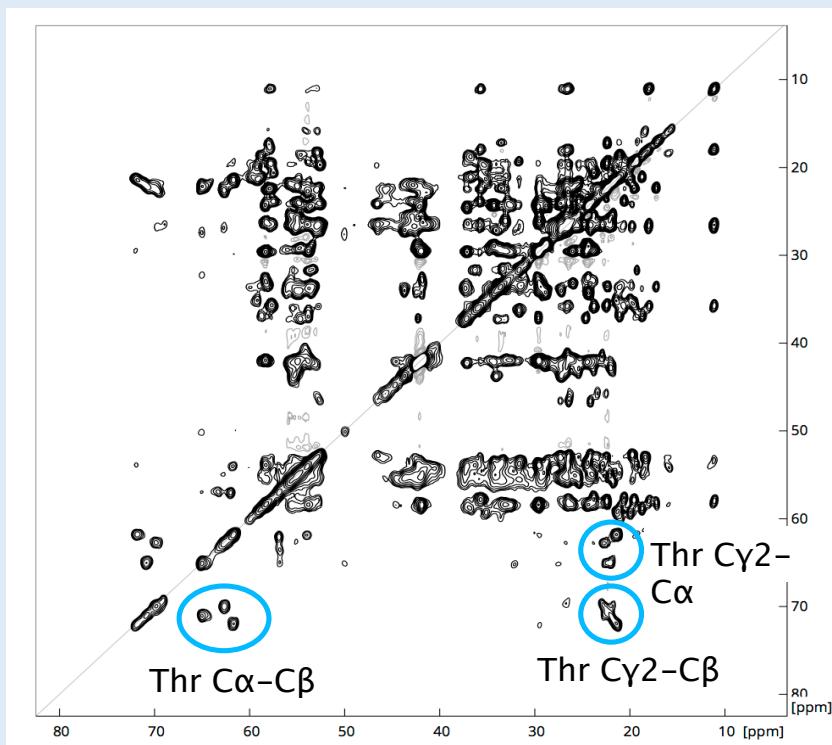
¹ Atoms reside in Residues, which reside in Chains; multiple chains can form a Complex.

² The id together with the type identifier forms the so-called pid, the project-identifier. As an example for an un-assigned CA in the 123rd NmrResidue in the second NmrChain: NA:@2..@123..CA. For an assigned NmrAtom, all the fields will have been filled, yielding something like NA:A.GLU.14.CA.

For more information see our video tutorial on NmrResidues at

<https://www.youtube.com/embed/DS9IZzNsBbQ>

Thr peaks in the PDSD sepctrum

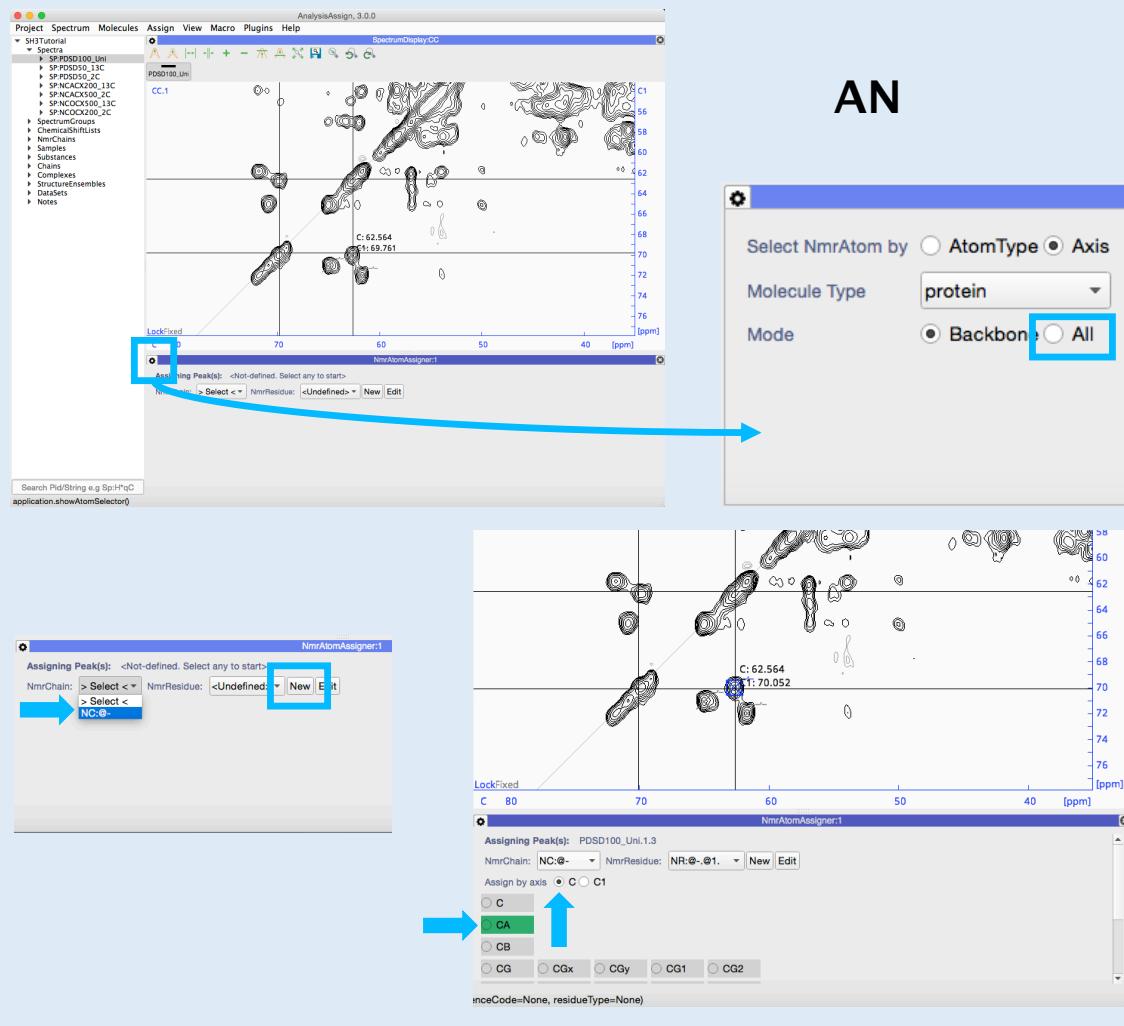
**3 A Identifying and peak picking the threonine residues**

Based on their characteristic chemical shifts, try to identify the $\text{C}\alpha\text{-C}\beta$, $\text{C}\alpha\text{-Cy}2$, $\text{C}\beta\text{-Cy}2$, $\text{C}\alpha\text{-CO}$ and $\text{C}\beta\text{-CO}$ cross peaks of the three threonines in the uniform (black) PDSD spectrum and peak pick them (except possibly the $\text{C}\beta\text{-Cy}2$ peaks which are not very well separated). Drawing marks through your peaks (**MK**) will help you connect them.

- Drag your PDSD100_Uni spectrum into the drop area and find the three $\text{C}\alpha\text{-C}\beta$ cross peaks below the diagonal ($x\text{-axis} \approx 63$ ppm; $y\text{-axis} \approx 71$ ppm).
- Begin by peak picking the left hand cross peak (**Shift+Ctrl/Cmd+left-drag**).
- Place a mark through this peak (**MK**).
- Look at the threonine $\text{Cy}2$ region at about 20 ppm. There is only one chemical shift (22.1 ppm) at which there are peaks which go through both marks (i.e. the $\text{C}\alpha\text{-Cy}2$ and $\text{C}\beta\text{-Cy}2$ cross peaks). Peak pick the $\text{C}\alpha\text{-Cy}2$ cross peak (22.1 and 65.0 ppm).
- Now go to the carbonyl region of the spectrum at around 170–180 ppm on the x -axis. Again there is one chemical shift (175.8 ppm) at which there are peaks which go through both marks. These are the $\text{C}\alpha\text{-CO}$ and $\text{C}\beta\text{-CO}$ cross peaks. Peak pick both of these. You have now identified one threonine spin system.

Now remove your marks (**MC**) and try the same procedure for the other two threonine spin systems.

Creating and assigning NmrAtoms and NmrResidues



3B Assigning NmrAtoms and NmrResidues

We will create NmrAtoms and NmrResidues using the NmrAtom Assigner:

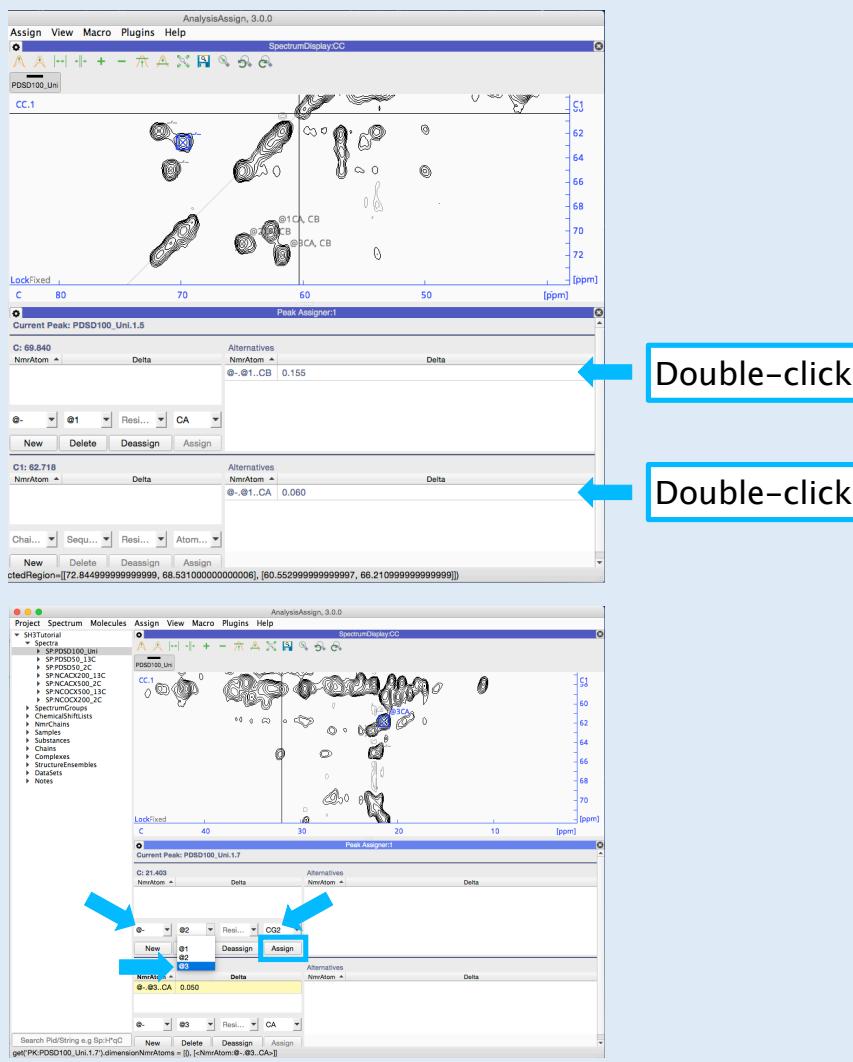
- Open the NmrAtom Assigner module with AN (or go to Main Menu → Assign → NmrAtom Assigner).
- Click on the gearbox icon () to change a setting: select Mode All (instead of Backbone). Click on the gearbox icon again to close the settings box.
- Select the NmrChain as @- from the pull down menu.
- Select a C α -C β cross peak below the diagonal and click on New in the NmrAtom Assigner. This will create a new NmrResidue @1 in NmrChain @-.

Now you need to assign each of the two dimensions of the peak to an atom type. In this case the C Axis corresponds to the C α chemical shift, and the C1 Axis to the C β :

- Select Assign by axis C and then click on CA.
- Select Assign by axis C1 and then click on CB.

Repeat this procedure for the other two C α -C β peaks.

Using the Peak Assigner



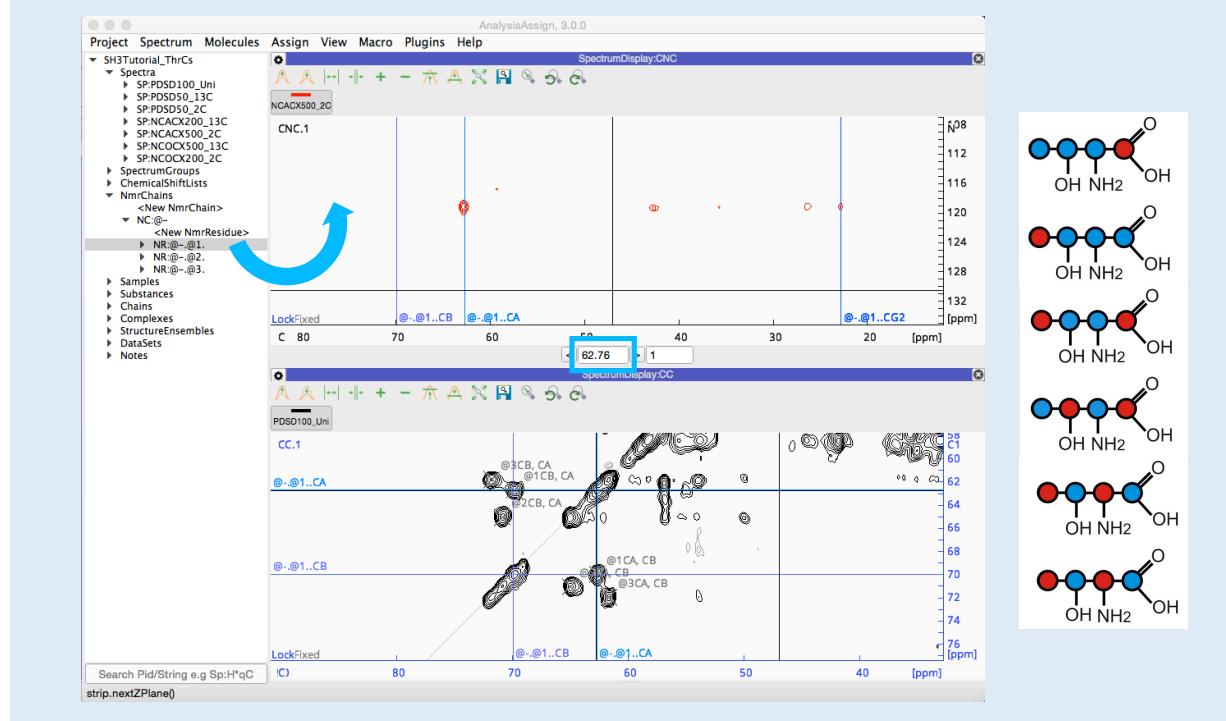
3C Assigning the remaining threonine peaks

For the remaining peaks it easiest to assign them using the Peak Assigner:

- Open the Peak Assigner with AP (or Main Menu → Assign → Peak Assigner).
- In the spectrum, select a C β -C α peak from above the diagonal. The Peak Assigner will now give you the CA and CB NmrAtoms as assignment options on the right hand side.
- **Double-click** both of these NmrAtoms in turn to assign them to the peak.
- Now select a C α -C γ peak.
- **Double-click** on the CA NmrAtom to assign it to the peak.
- For the C γ dimension, change the NmrChain and NmrResidue to be the same as that of the CA NmrAtom and change the atom name to **CG2**.
- Click **Assign** to make this assignment to the peak.

Repeat this process for the other C α -C γ peaks and then do the equivalent for the C α -C' and C β -C' peaks, selecting C as the carbonyl atom name.

Identifying Thr peaks in the NCACX



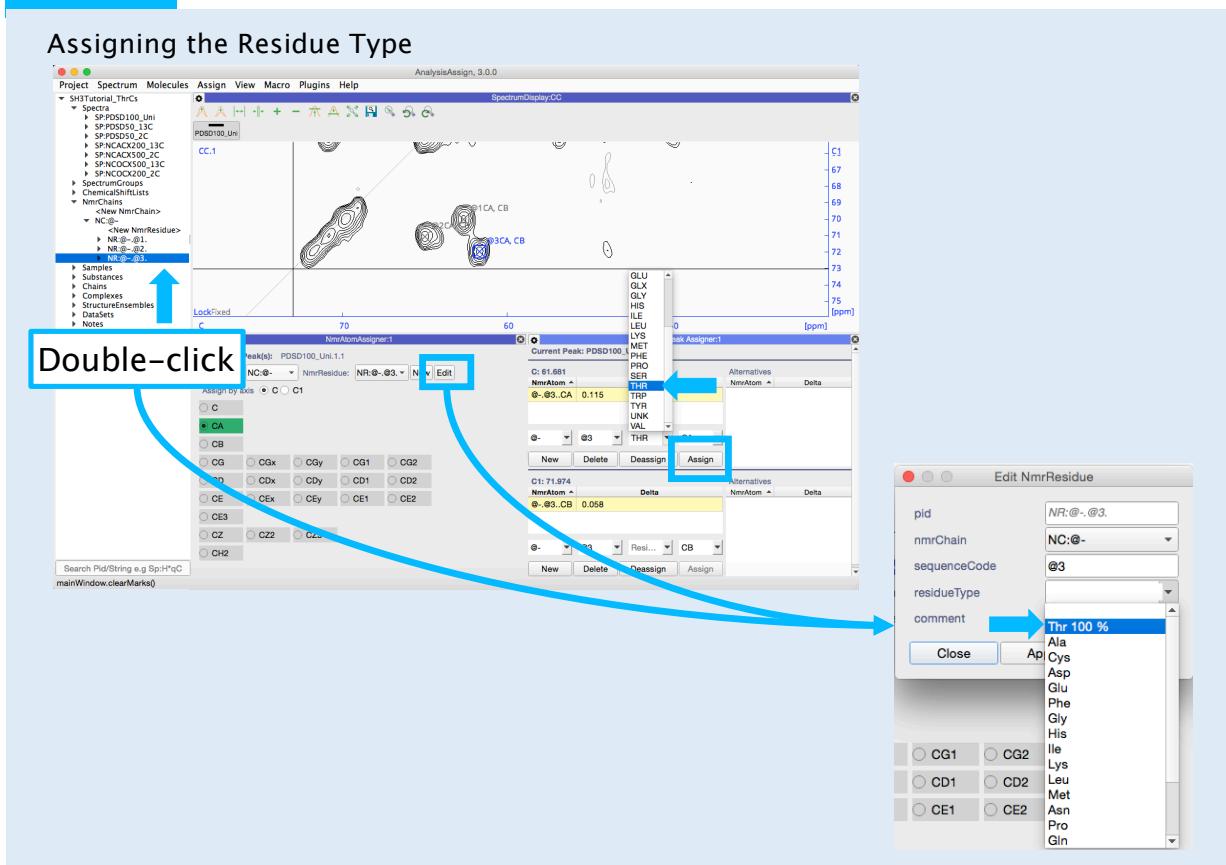
3D Assigning the threonine nitrogen chemical shifts

Now we will identify the threonine nitrogen chemical shifts using the NCACX500_2C spectrum:

- **Drag** the NCACX500_2C spectrum into the drop area.
 - Type **YZ** to swap the Y and Z axes so that the CA dimension lies along the z-axis. You may want to rearrange your display modules as above now.
 - In the sidebar, expand **NmrChains** and **NmrChain NC:@-**.
 - **Drag** one of the threonine NmrResidues into the drop area. This will draw marks at the positions of this NmrResidue's NmrAtoms.
 - Type the C α chemical shift of this NmrResidue into the z-axis position of the 3D display. You should find a strip which contains a strong N-C α -C α 'diagonal' cross peak as well as a slightly weaker N-C α -C γ cross peak.
- Looking at the glycerol labelling scheme you will see that N-C α -CO and N-C α -C β cross peaks should not be observable for a threonine in the NCACX spectrum of the 2- ^{13}C glycerol sample, as the C α and CO or C α and C β are never simultaneously labelled.

Peak pick your N-C α -C γ cross peaks and assign the nitrogen chemical shifts using the procedure you used previously for the carbon resonances:

- Bring up the Peak Assigner with **AP**.
- **Double-click** on the C α and C γ resonances suggested as assignment options. In the nitrogen dimension, select the correct NmrChain, NmrResidue and **N** as the atom.
- Click on **Assign** to make the assignment.



3E Assigning the Residue Type

From the chemical shifts we know that the spin systems, or NmrResidues that we have assigned are threonine residues, so we can also assign the amino acid type. There are several ways in which this can be done:

- **Double-click** on an NmrResidue in the sidebar to bring up the **Edit NmrResidue** popup.
- Select the residue type from the drop-down menu and click **Okay**.

OR

- Select a threonine peak.
- Open the Peak Assigner with **AP**.
- In one of the dimensions, select the residue type from the drop-down menu and click **Assign**.

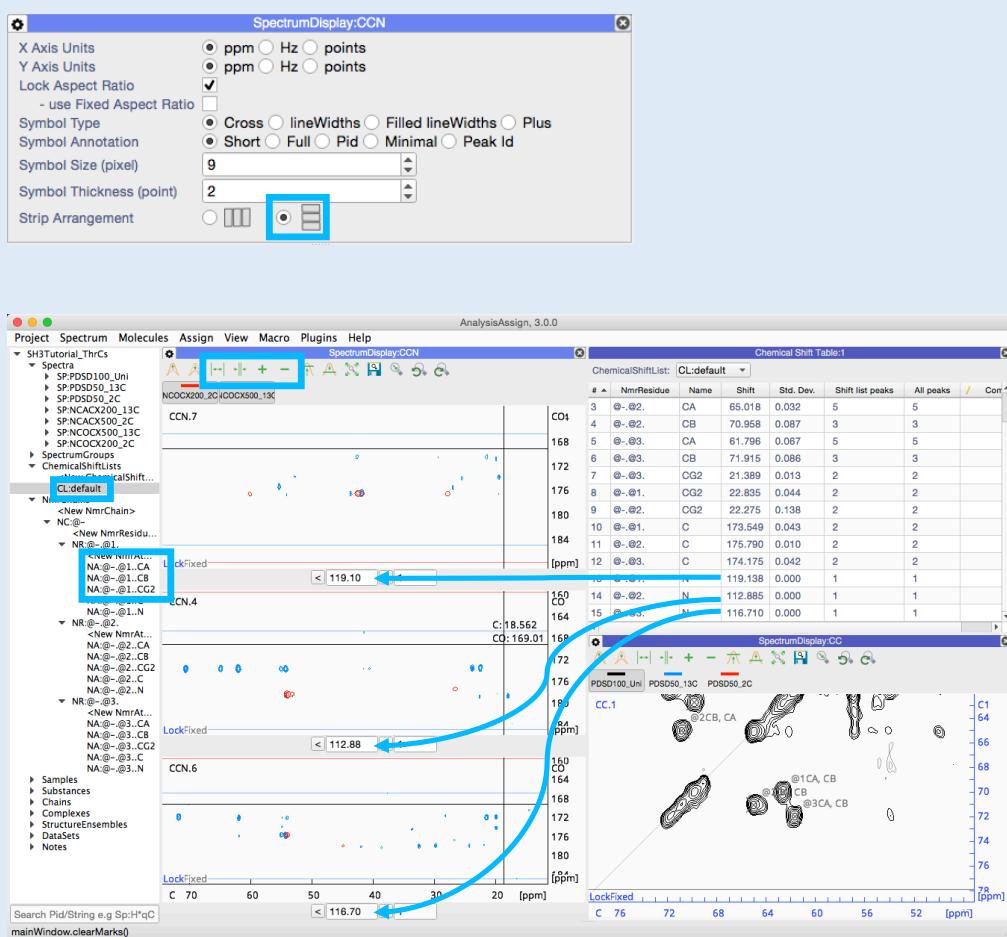
OR

- Select a threonine peak.
- Open the NmrAtom Assigner with **AN**.
- Click on **Edit** to bring up the **Edit NmrResidue** popup.
- Select the residue type from the drop-down menu and click **Okay**.

Repeat for all three threonine residues.

The assignment of the residue type can be done at any stage, i.e. you could have done this as part of one of the previous steps if you had wanted.

Setting up Horizontal Strips

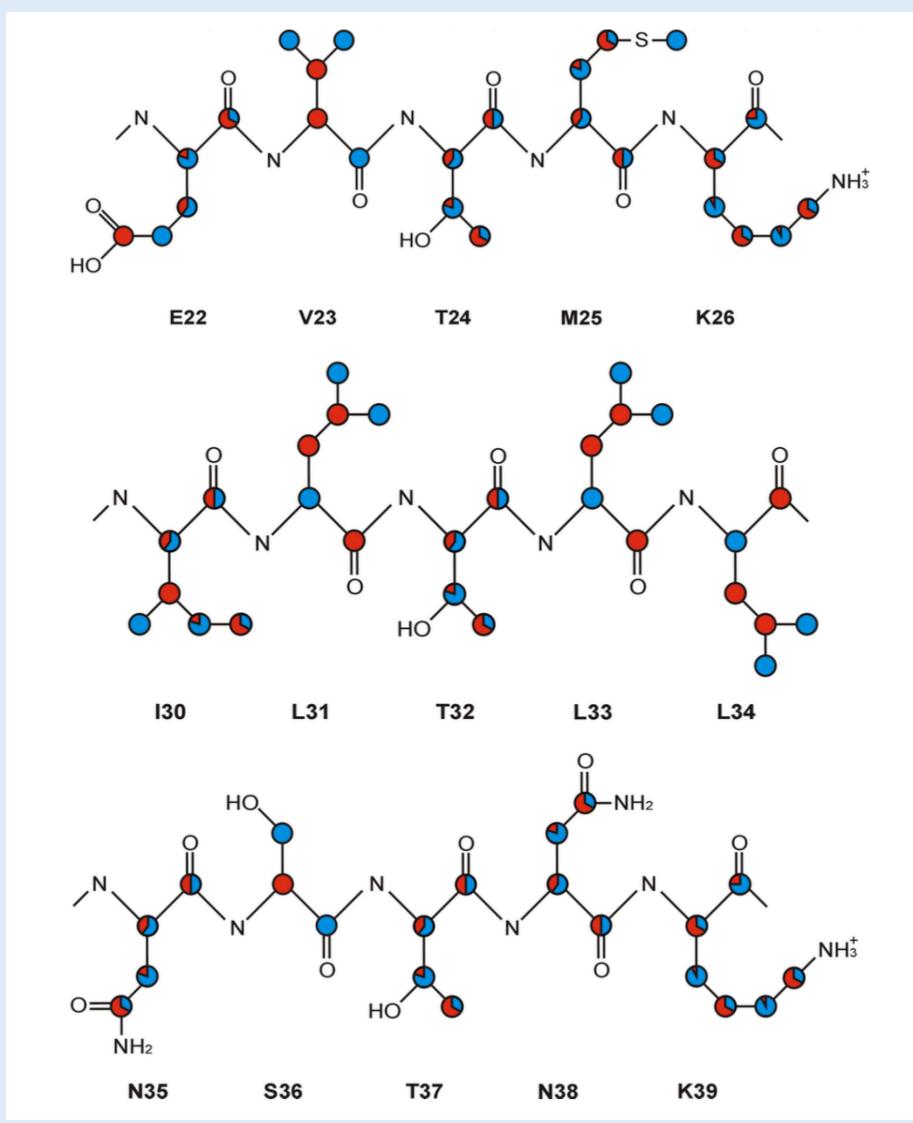


4A Setting up horizontal strips

We will now use horizontal strips to look at all three threonines in parallel:

- Drag your NCOCX500_13C and NCOCX200_2C spectra into the drop area.
- Click on the gearbox icon () to change a setting: select **Strip Arrangement** and click on the gearbox icon again to close the settings box.
- Now add two strips clicking on the + icon in the Spectrum Display toolbar.
- If necessary, narrow the strips with so you can see all three strips properly.
- Expand the Chemical Shift Lists in the side bar and drag the chemical shift list into the drop area.
- Set the z-plane Nitrogen positions of your NOCOX strips to those of your three threonines.
- You can mark the aliphatic NmrAtoms of each threonine in turn by dragging the NmrResidue from the sidebar into the drop area. Use MC to clear the marks again.

Glycerol labelling pattern of Thr motifs in the SH3 domain

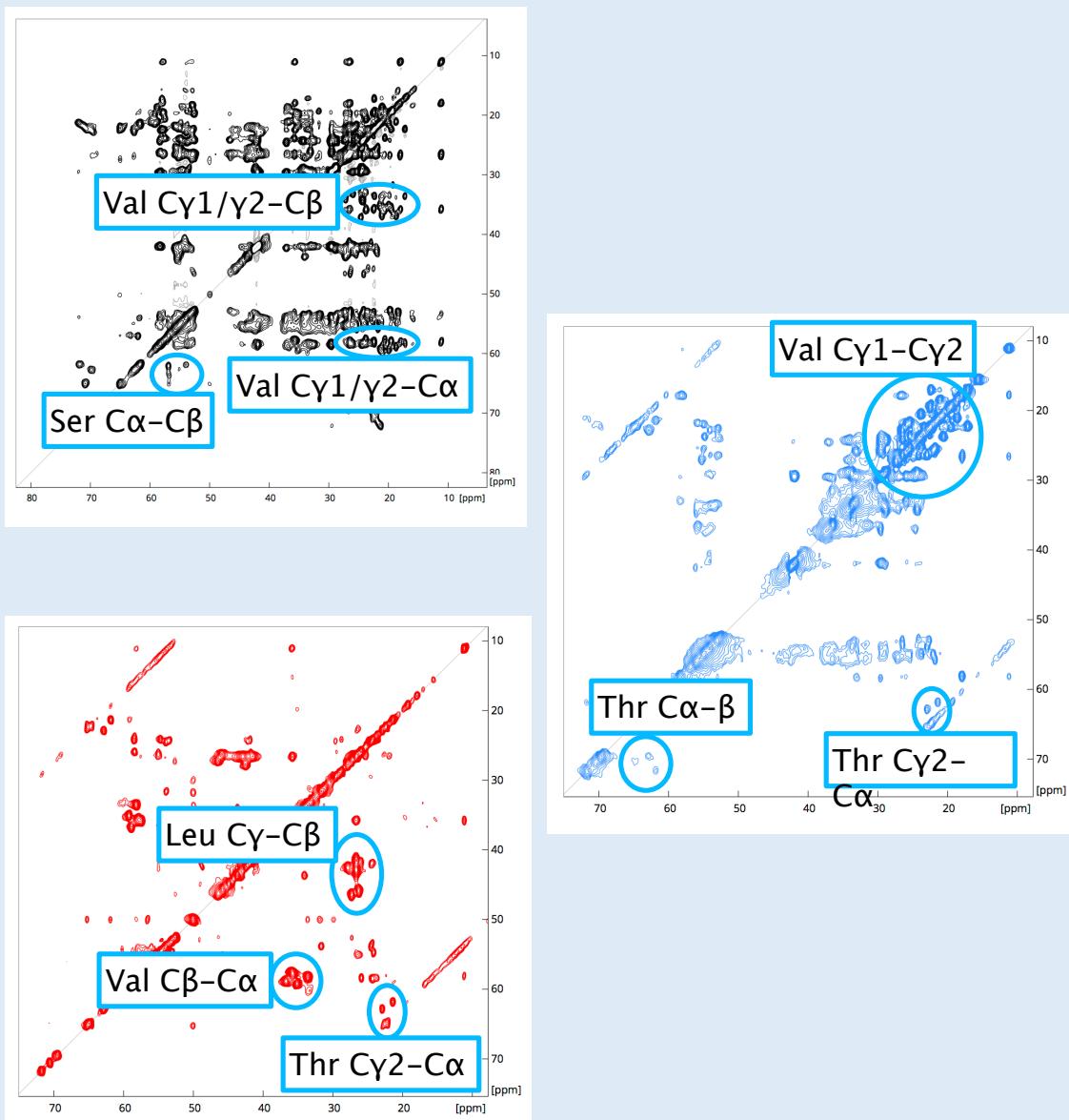


4B Identifying the residues preceding the threonines

Using the NCOCX500_13C and NCOCX200_2C spectra, the glycerol labelling pattern and the standard chemical shifts it is possible to work out which threonine is preceded by a valine, which by a leucine and which by a serine:

- In the nitrogen plane of the threonine which is preceded by a valine, you should only be able to see cross peaks in the NCOCX spectrum of the 1,3-¹³C glycerol sample. The Cy resonances of a valine (~ 20 ppm) and the C α , C β , possibly also Cy2 resonance of your threonine should be visible.
- For the threonine preceded by the leucine, you should only see peaks in the 2-¹³C glycerol sample: the C β and Cy resonances of a leucine (~42 and ~27 ppm, respectively) and the C α , perhaps also C β and Cy2 of the threonine.
- For the threonine preceded by a serine, cross peaks will again only be visible in the 1,3-¹³C glycerol sample: The C β of the serine (~ 64 ppm) and the C α , C β , possibly also Cy2 resonance of your threonine.

Val, Ser and Leu patterns in C-C spectra

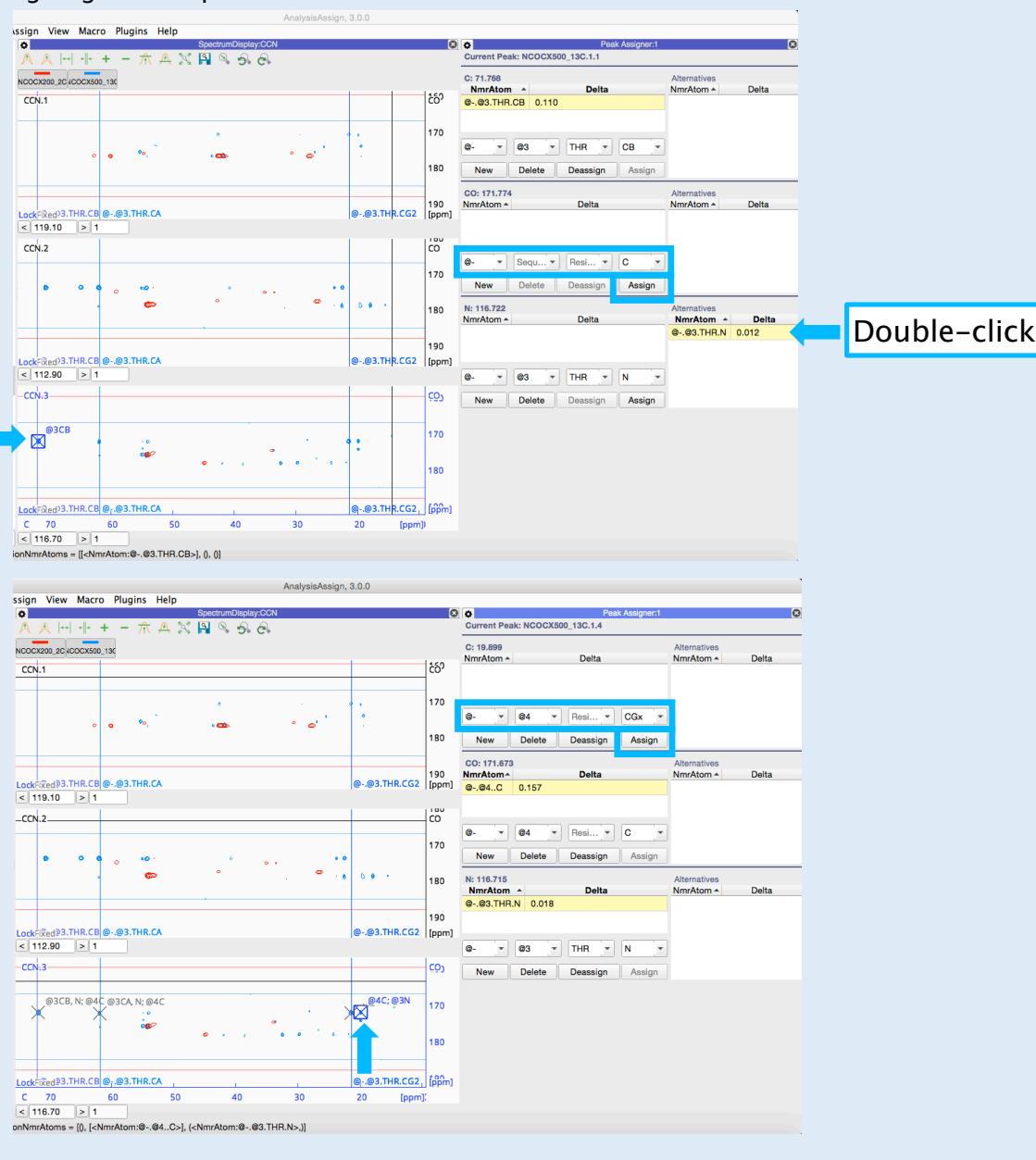


4C Confirming your assignment of the preceding residues

You can confirm whether the peaks which you think may arise from valine/leucine/serine residues really do, by marking them and checking whether you can see any corresponding cross peaks in the PDSD spectra.

- For valine you should see a Cy1-Cy2 cross peak (near the diagonal at ~ 20 ppm) in the 1,3-¹³C glycerol spectrum and Cy1/2-Cα (~ 20/62 ppm) and Cy1/2-Cβ (~ 20/33 ppm) cross peaks in the uniformly labelled spectrum and a strong Cα-Cβ cross peak (~ 62/33 ppm) in the 2-¹³C glycerol spectrum.
- For leucine your Cβ and Cy should form a strong cross peak in the 2-¹³C glycerol spectrum (~ 42/27 ppm).
- For serine you would expect a Cα-Cβ cross peak (~ 58/64 ppm) in the uniformly labelled spectrum.

Assigning NCOCX peaks



4 D Assigning the NCOCX peaks

In order to assign the cross peaks in the 3D NCOCX spectra,

- bring up the Peak Assigner by typing AP and select each peak in turn.

For the N and CX dimensions your threonine NmrAtoms should be provided as assignment options.

- Double-click** these to assign them to your peak.

This leaves the C' dimension which belongs to the previous residue.

- Select your default NmrChain @-, and the atom type C and then click **Assign**.

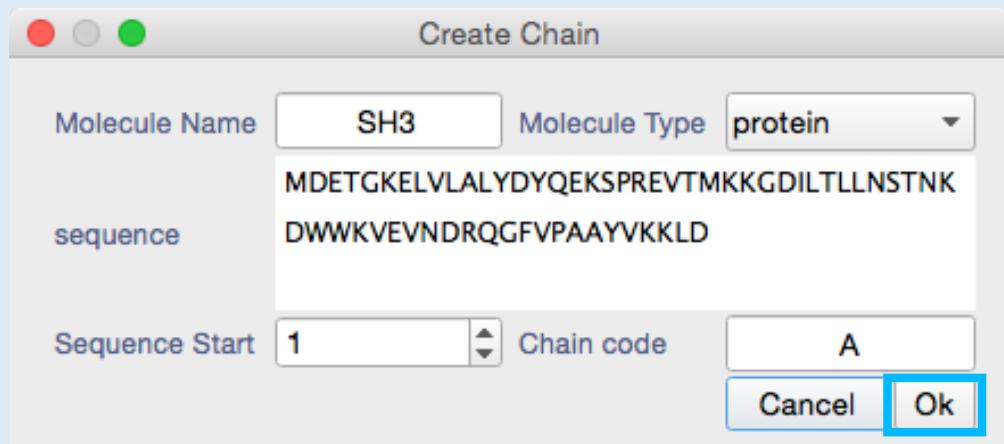
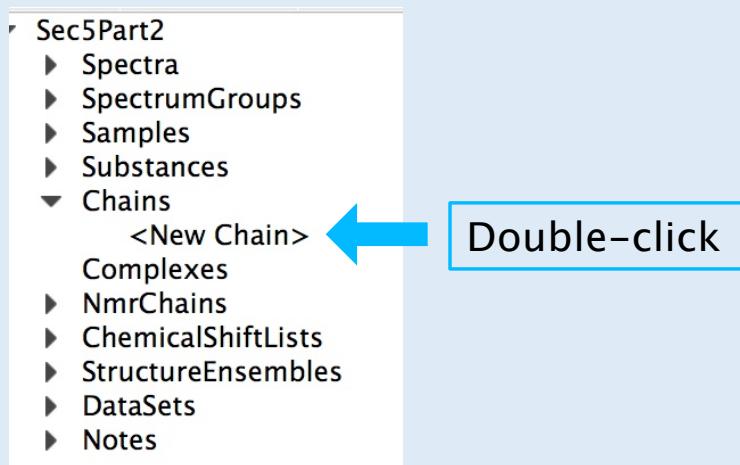
The program will automatically create a new NmrAtom and NmrResidue.

Use this same new NmrResidue when assigning further peaks. When assigning the Val Cy peaks, use CGx and CGy as the atom names, as the assignment is non-stereo specific. You can also assign the Val, Leu and Ser residue types.

5 Sequence Specific Assignments

Sec5Part1

Add a new Protein Chain



5A Create chain

To make sequence-specific assignments you will need to add the sequence of the SH3 domain to your project:

- Sidebar → Chains → <NewChain>
- followed by
- Molecule Name: SH3
- ChainCode: A
- Sequence: (copy and paste)
MDETGKELVLALYDYQEKS...
DWWKVEVNDRQGFVPAAYVKL...
DWWKVEVNDRQGFVPAAYVKL...
- click Ok

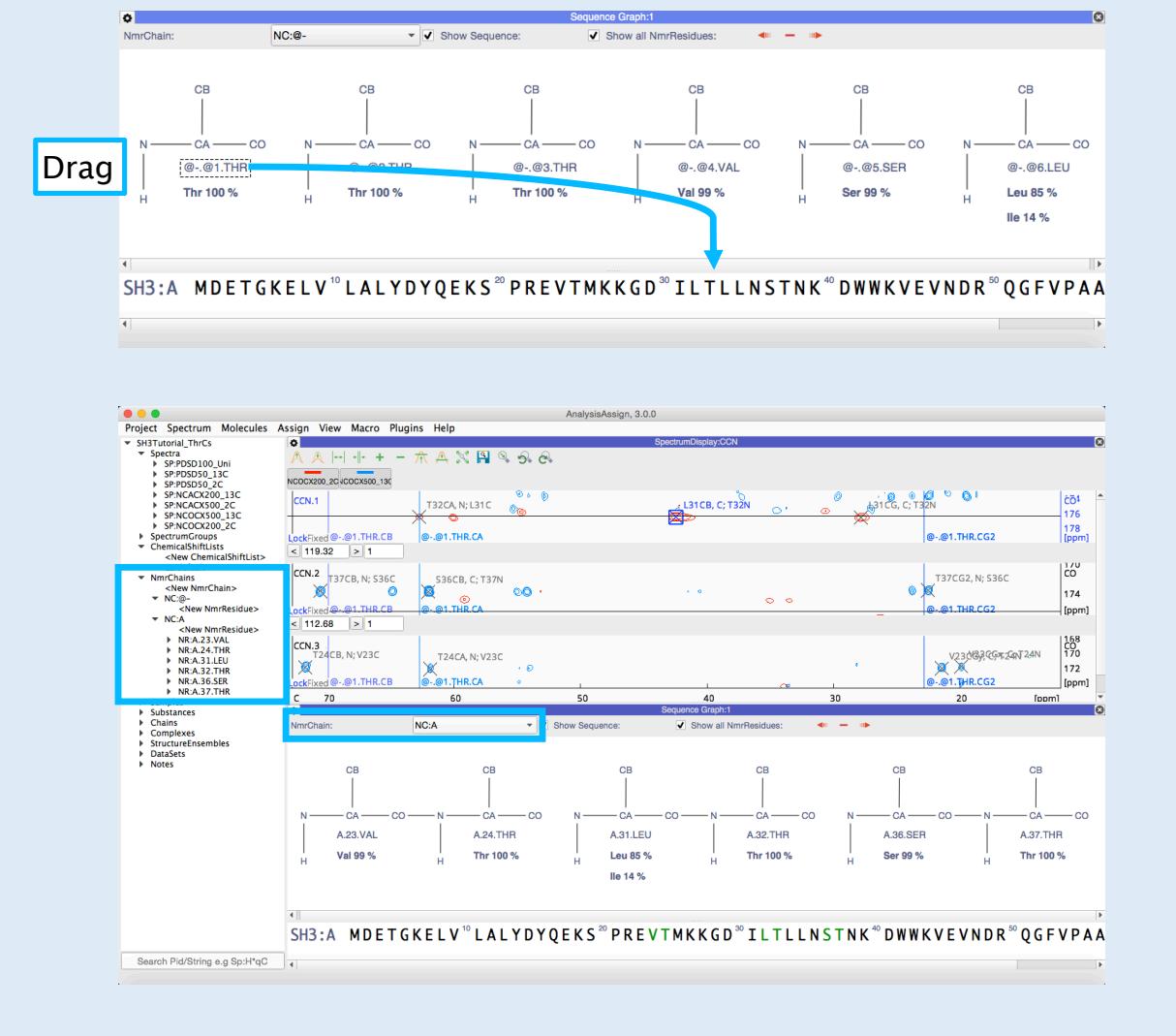
You can also use Main Menu → Molecule → Generate Chain or drop a FASTA formatted file into the project.

5 Sequence Specific Assignments

SH3Tutorial

Sequence-specific Assignment

SG



5B Making sequence-specific assignments

Bring up the Sequence Graph:

- Go to Main Menu → View → Sequence Graph or type SG.

You will see all your NmrResidues in the upper panel and the protein sequence below.

- Drag an NmrResidue from the upper panel onto the residue in the sequence below that you want to assign it to.

This residue in the sequence will now turn green to show that it is assigned.

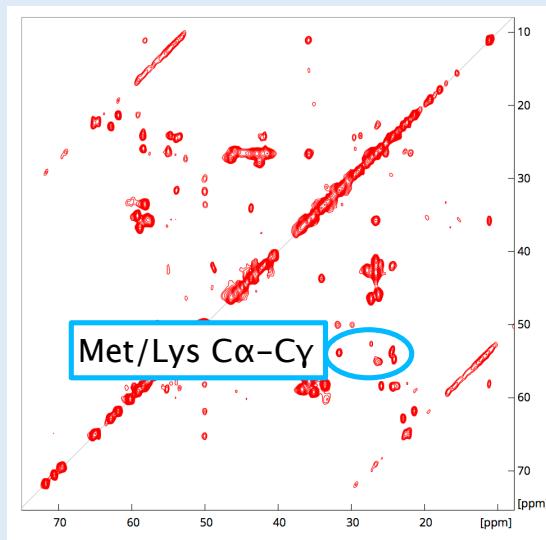
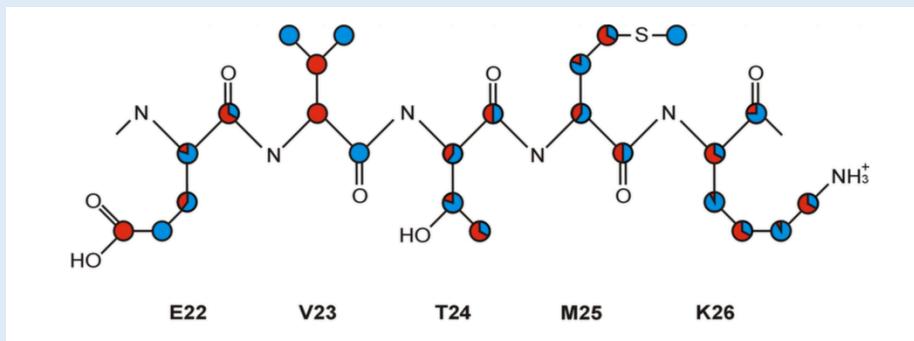
The assigned NmrResidues are placed into a new NmrChain called A to show that they are assigned to the Residues in Chain A. This is reflected in the sidebar.

When you have assigned all your NmrResidues,

- select NmrChain NC:A in the Sequence Graph.

You will see all your NmrResidues again and can see that sequential residues are shown as being linked.

EVTMK Motif in the SH3 domain

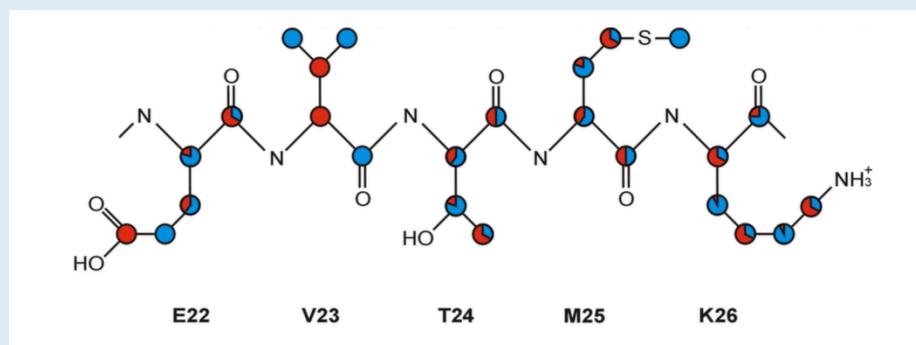
**6A Further assignment of the EVTAK motif – linking to the methionine**

Try to identify the methionine which follows this threonine.

Use the NCOCX200_2C spectrum with C' in the Z-dimension and go to the plane of the threonine C'. You should be able to see links to the threonine C β and methionine C α . To confirm that the C α you have found really is compatible as a methionine C α – see if it matches up with a possible C α -C γ cross peak in the 2- ^{13}C glycerol PDSD spectrum. You should be able to confirm the nitrogen chemical shift of the methionine residue by looking for the N-C α -C γ peak in the 2- ^{13}C glycerol NCACX.

At each stage, pick your peaks and assign your NmrAtoms and NmrResidues.

EVTMK Motif in the SH3 domain



Peak Assigner:1

Double Tolerances Only Intra-residual Allow Multiple Peaks Peak Selection from Table

Current Peak: NCACX500_2C.1.4

C: 31.595 NmrAtom ▲	Delta	Alternatives NmrAtom ▲	Delta
A.25.MET.CG	0.029		
<hr/>			
A ▾ 25 ▾ MET ▾ CG ▾			
New	Delete	Deassign	Assign

C1: 53.790 NmrAtom ▲	Delta	Alternatives NmrAtom ▲	Delta
A.25.MET.CA	0.028		
<hr/>			
A ▾ 25 ▾ MET ▾ CA ▾			
New	Delete	Deassign	Assign

N: 121.442 NmrAtom ▲	Delta	Alternatives NmrAtom ▲	Delta
		A.25.MET.N	0.408
<hr/>			
A ▾ 25 ▾ MET ▾ N ▾			
New	Delete	Deassign	Assign

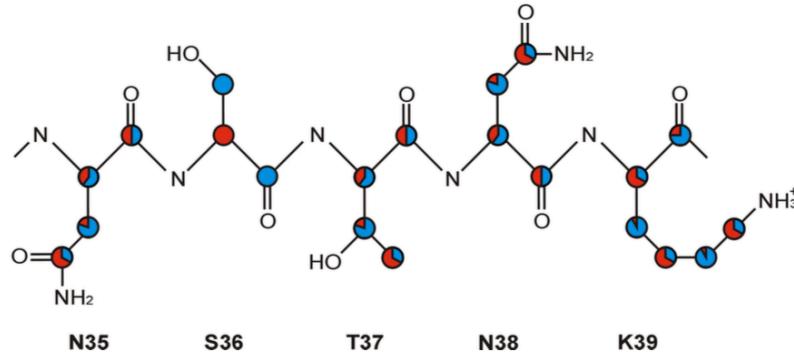
6B Further Assignment of the EVTMK motif – linking to the Lysine

Now see if you can find links from the methionine to the neighbouring lysine. First find the Met C' and C β chemical shifts via the C γ -C' and C γ -C β peaks in the PDSD100_Uni spectrum. Then find the Lys N and C α in the NCOCX200_2C spectrum. You can confirm that you have identified the correct resonances/peaks (and eliminate incorrect resonances/peaks) by looking for a matching Lys C α -C γ peak in the PDSD50_2C spectrum and a Lys N-C α -C γ peak in the NCACX500_2C spectrum.

If you are expecting to see an NmrAtom as an option in the Peak Assigner and it is now shown, try extending the matching tolerance:

- Go the **Settings** box of the **Peak Assigner** by clicking on the gearbox icon
- Tick the **Double Tolerances** box

NSTNK Motif in the SH3 domain



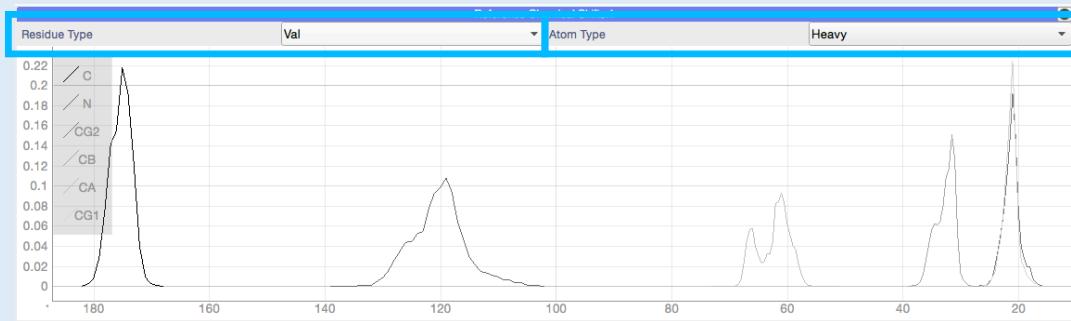
6C Further Assignment of the NSTNK motif

If you have got to this stage, then you have probably got the hang of things.

Try identifying the remaining resonances of the serine spin system and see if you can find links to the preceding asparagine.

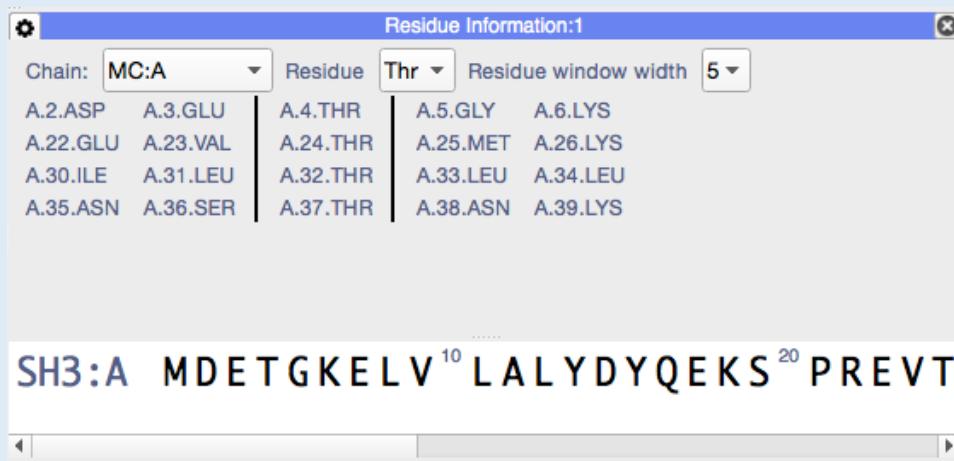
Use the tools in section 7 to help you find the serine and asparagine reference chemical shifts and correct mistakes.

Reference Chemical Shifts



RC

Residue Information



RI

7 A Reference Chemical Shifts

You can check the standard chemical shifts for protein amino acids within CcpNmr Analysis:

- Go to **Main Menu → Molecules → Reference Chemical Shifts**, or type **RC**.
- Select the **Residue Type** and **Atom Type** of your choice.

7 B Residue Information

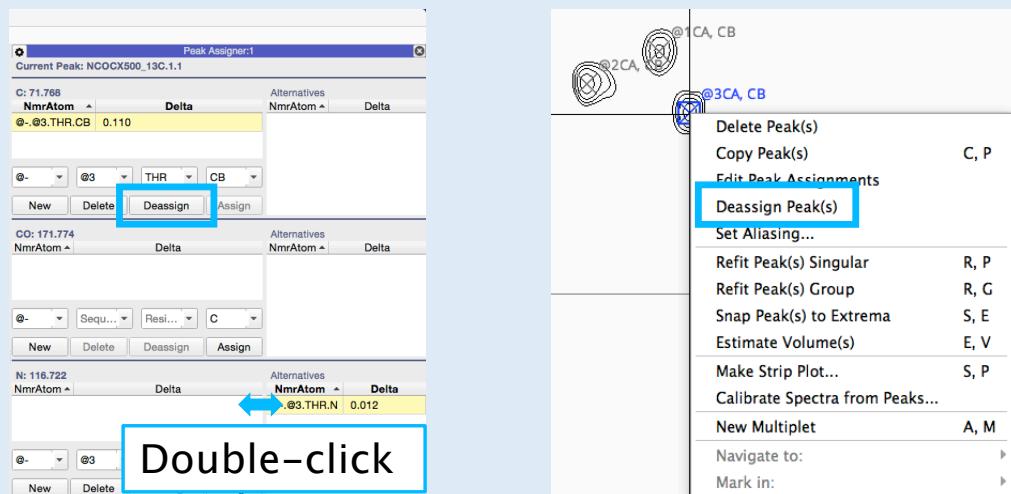
You can look at different residue types in your sequence and the motifs they are contained in:

- Go to **Main Menu → Molecules → Residue Information**, or type **RI**.
- Select the **Chain**, **Residue Type** and **Residue Window Width** of your choice.

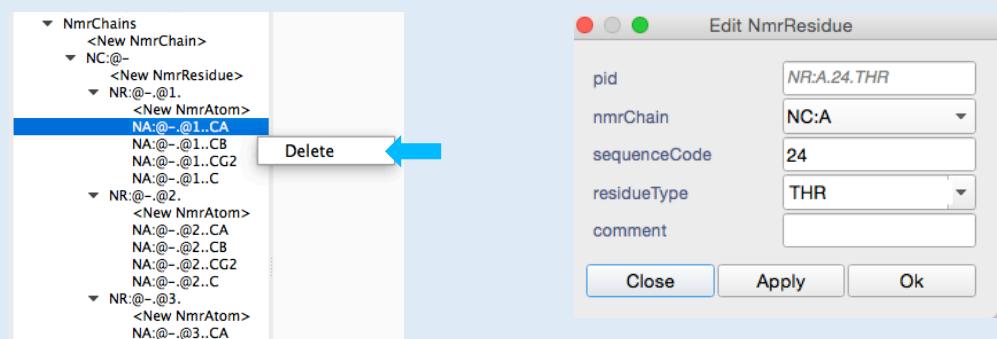
The full sequence is shown below and if you have made any sequence specific assignments, then these residues will be highlighted in green.

You will notice that the SH3 domain actually has four threonines. The first of these, is highly mobile and not visible in the spectra used here.

De-assigning Peaks



Changing NmrAtom / NmrResidue Assignments



7C Removing an assignment from a peak

You can do this via the Peak Assigner (AP):

- Click the **Deassign** button to remove an NmrAtom assignment
- This will move the NmrAtom from the left hand side (assignment) to the right hand side (assignment options) of the Peak Assigner module **OR**
- Double-click** on an NmrAtom to move it from one side to the other **OR**
 - Right-click** on one or more peaks in a spectrum and select **Deassign Peak(s)**
- This will remove the assignments from the peak in all dimensions.

7D Changing the assignment of an NmrAtom or NmrResidue

To delete an NmrAtom or NmrResidue:

- Right-click on one or more NmrAtoms or NmrResidues in the sidebar and select **Delete**

To change the assignment of an NmrAtom or NmrResidue:

- Double-click** on NmrAtoms/NmrResidues in the sidebar to bring up an **Editor**
- Enter your new assignment and click **Okay**.

Note that you don't have to use the drop-down menus. You can also enter free text into the boxes. An NmrResidue could be called '24/35/44' if you are not sure of the assignment.

Contact Us

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<https://www.ccpn.ac.uk/forums>

Cite Us

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Tutorial Version History:

3.0 (VAH): First version