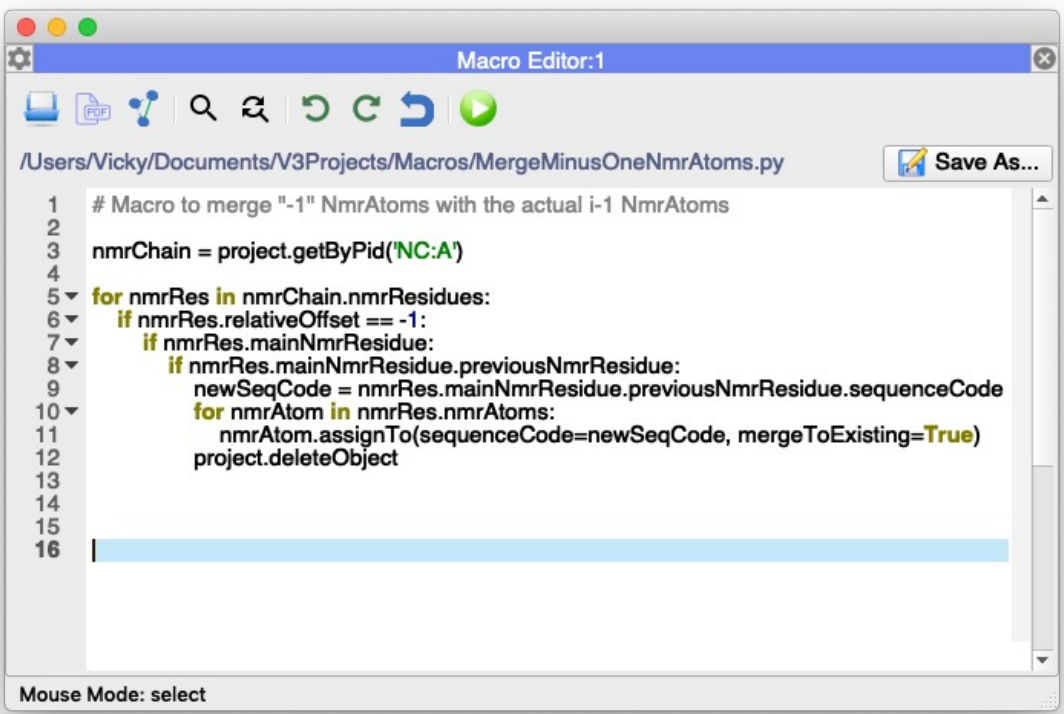
CCPN

CcpNmr AnalysisScreen Version 3

Macro Writing Tutorial



Introduction

This tutorial is designed to introduce you to macro writing in CcpNmr Analysis 3.1. It begins by taking you through some basic concepts in object oriented programming and the CcpNmr Analysis data structure. This is followed by a series of worked examples and problems which gradually increase in complexity.

It is assumed that you have some basic familiarity with the CcpNmr Analysis programme (e.g. from having completed our Beginners Tutorial). It will also help if you have some basic knowledge of Python programming (e.g. indentations, conditionals and loops).

You can use your own NMR data or that located in the **/CcpnTutorialDataMacroWritingApril22** directory provided by CCPN.

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

Contents:

Start CcpNmr Analysis V3

Apple users by double-clicking the *CcpNmrAnalysis* icon

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

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

1 CcpNmr Analysis data structure

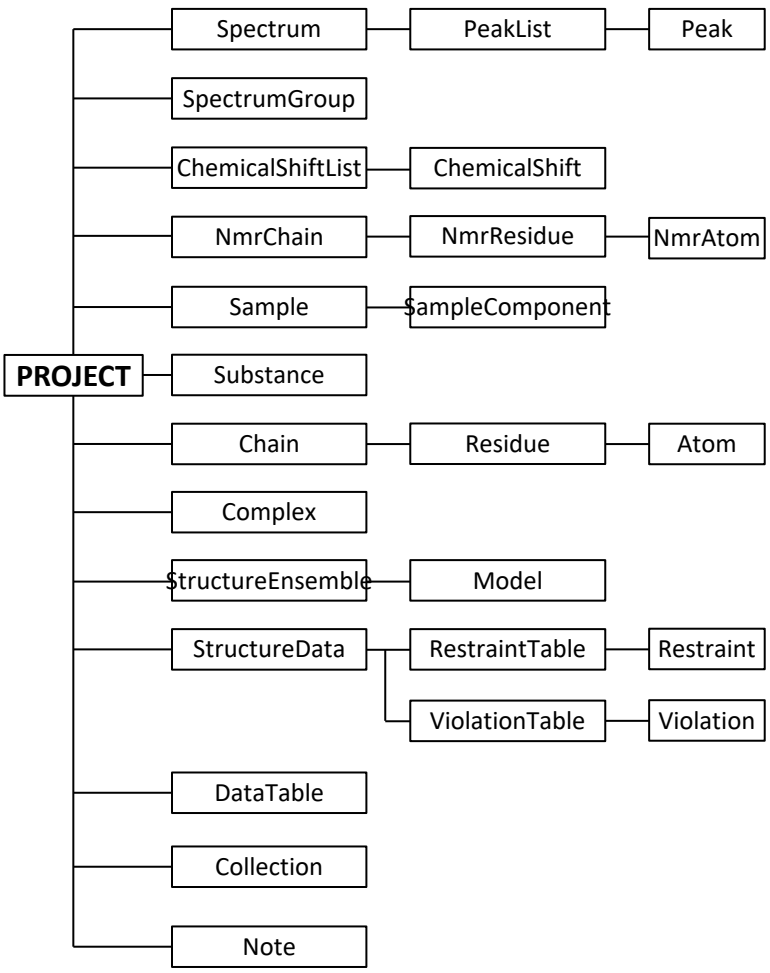
Classes, objects, methods and properties in CcpNmr Analysis V3

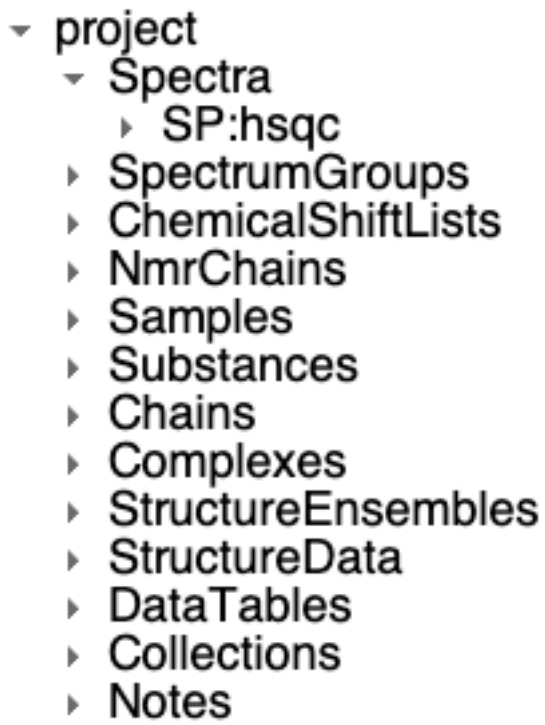
(Explanation only)

The main types of data contained within Analysis are shown below (left). Some of these are nested within each other, e.g. a peak **is always contained within a** peak list **and a** peak list **is always associated with a** spectrum**. The data structure of the programme is reflected in the way the data is shown in the sidebar of Analysis (right).**

Each data type forms a so-called class **within the programme. Actual pieces of data within these classes are referred to as** objects**. Each** class **has a variety of** properties **(think of them as variables) and** methods **(essentially subroutines or functions) associated with it, i.e. different types of data (e.g. spectra, peak lists, peaks, chemical shifts, NmrAtoms etc.) automatically have certain properties and methods associated with them. For example,** spectrum.name **(a property) would give you the name of a spectrum and** spectrum.rename(value='HSQC') **(a method) would change your spectrum's name to** HSQC**.**

Thus, if you want to write a macro, there are a large number of routines that you can draw on to access and manipulate all the data in your project. The tutorial will show you how to find and use these routines to change or display your data as you would like.





1 CcpNmr Analysis data structure

Project IDs (Pids)

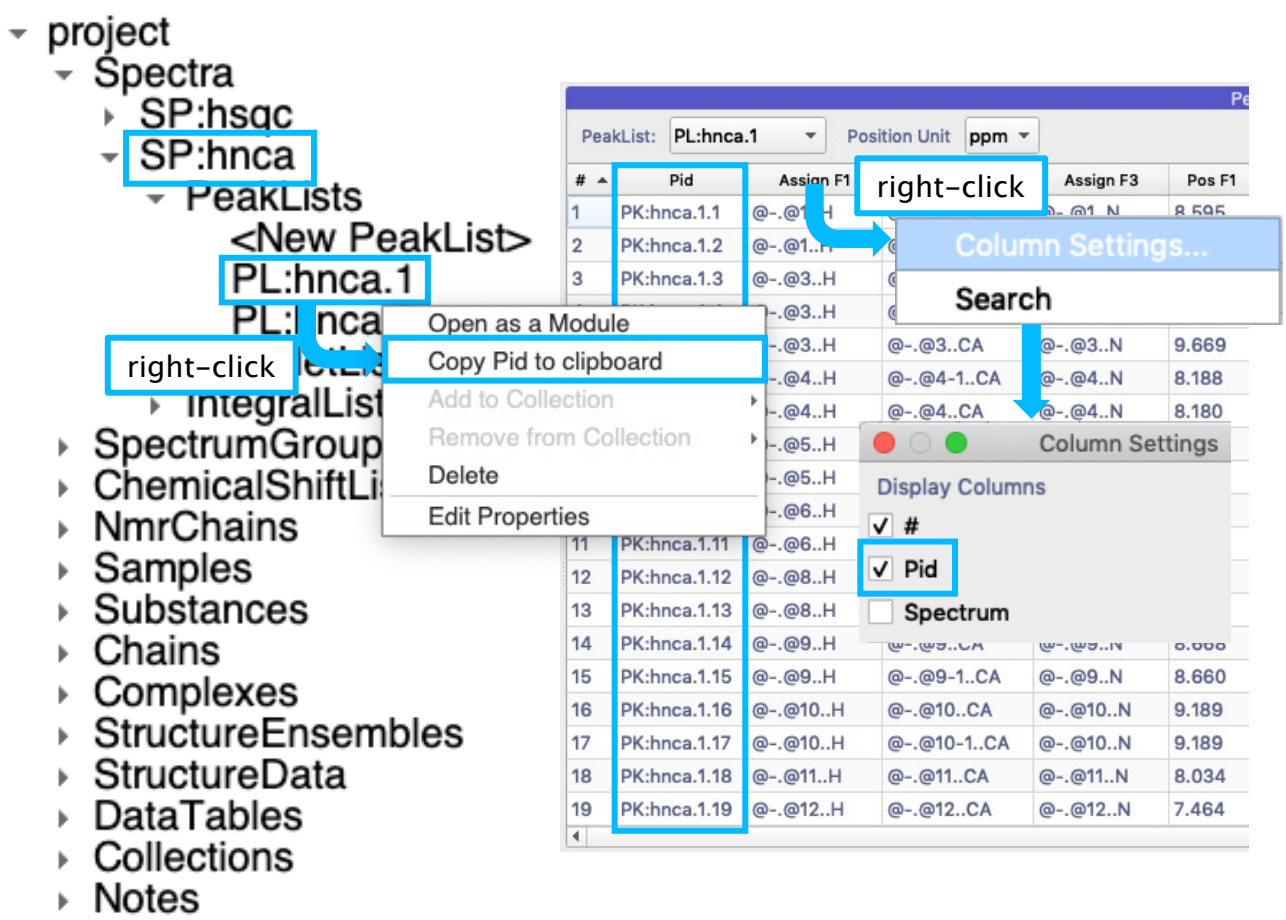
(Explanation only)

Each object within Analysis has its own unique Project ID **(or PID/Pid). These Pids contain a short code to signify the data type (e.g.** SP **for spectrum – see next page for a full list) followed by the name of the data item, e.g.** SP:hsqc**. Nested items also contain the names of their parents/grandparents, separated by a full stop. For example, the PID of a peak list is given as** PL:spectrumName.peakListName **or of an NmrAtom as** NA:A.23.THR.CA**.**

These Pids are very useful during macro writing for getting hold of particular items of data. You will see in Section 2C that get('Pid') **will give you the object with that Pid for you to do something with (e.g. execute a method on, assign to a variable etc.).**

You can easily find an object's Pid, as they are all shown in the sidebar and you can also view them in tables. You can also copy them to the clipboard via the right-hand mouse menu.

A full list of PIDs with examples is given on the next page.

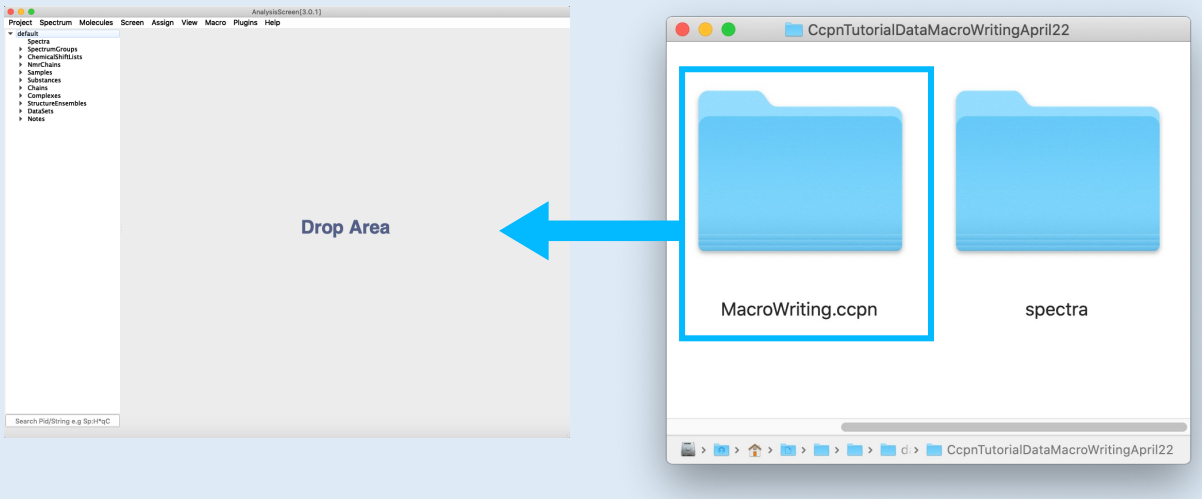


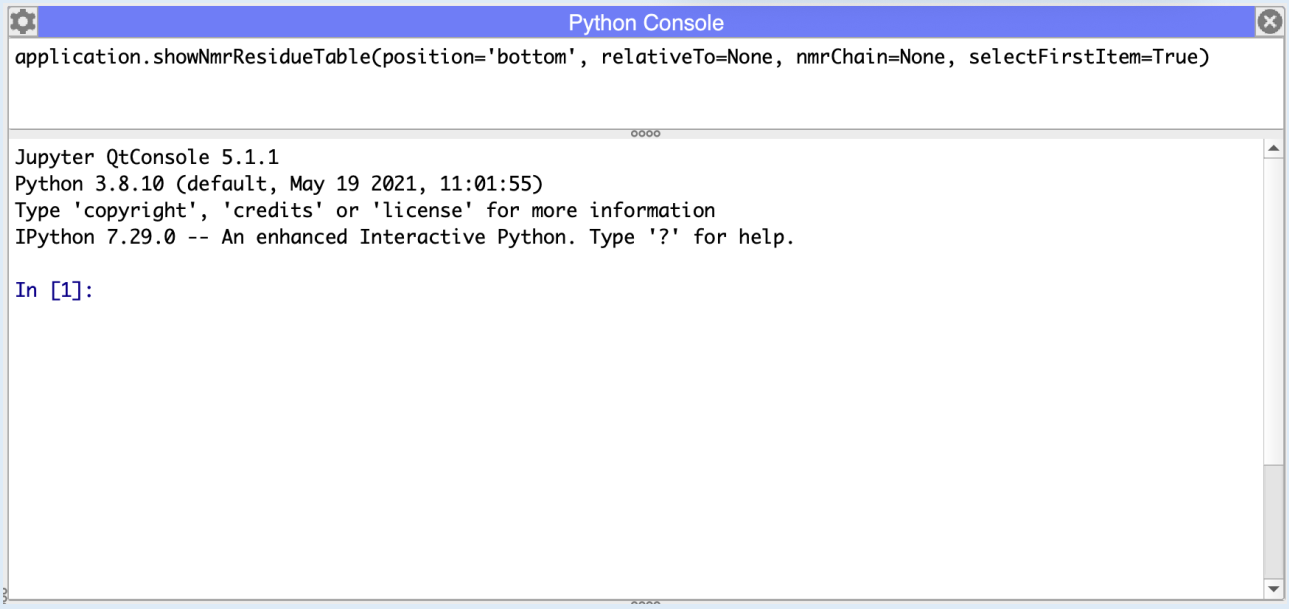
1 CcpNmr Analysis data structure

Project IDs in Analysis

PID Short Code	Data Object	Nesting	Example
PR	Project	Project	PR:GP41fab8066Complex
SP	Spectrum	Spectrum	SP:hsqc
PL	Peak List	Spectrum / Peak List	PL:hsqc.1
PK	Peak	Spectrum / Peak List / Peak	PK:hsqc.1.1
ML	Multiplet List	Spectrum / Multiplet List	ML:hsqc.1
MT	Multiplet	Spectrum / Multiplet List / Multiplet	MT:hsqc.1.1
IL	Integral List	Spectrum / Integral List	IL:hsqc.1
IT	Integral	Spectrum / Integral List / Integral	IT:hsqc.1.1
SG	Spectrum Group	Spectrum Group	SG:T1Data
CL	Chemical Shift List	Chemical Shift List	CL:default
CS	Chemical Shift	Chemical Shift List / Chemical Shift	CS:default.A.23.THR.H
NC	NmrChain	NmrChain	NC:A
NR	NmrResidue	NmrChain / NmrResidue	NR:A.23.THR
NA	NmrAtom	NmrChain / NmrResidue / NmrAtom	NA:A.23.THR.CA
SA	Sample	Sample	SA:complex
SC	Sample Component	Sample / Sample Component	SC:complex.GP41
SU	Substance	Substance	SU:GP41
MC	(Molecule) Chain	Chain	MC:A
MR	(Molecule) Residue	Chain / Residue	MR:A.23.THR
MA	(Molecule) Atom	Chain / Residue / Atom	MA:A.23.THR.H
MX	(Molecule) Complex	Complex	MX:GP41-fab8066
SE	Structure Ensemble	Structure Ensemble	SE:4kht
SD	Structure Data	Structure Data	DS:run1
RT	Restraint Table	Structure Data / Restraint Table	RT:run1.TalosRestraints
RE	Restraint	Data Set / Restraint List / Restraint	RE:run1.TalosRestraints.1
DT	Data Table	Data Table	DT:RamachandranData
CO	Collection	Collection	CO:run1
NO	Note	Note	NO:note1
GS	GUI Strip	GUI Strip	GS:2D_HN.1

2 Using the Python Console





2A Open Spectra/Project

- **Drag** the **CcpnTutorialDataMacroWritingApril22/MacroWriting.ccpn** project into the Drop Area.

2B Open Python Console

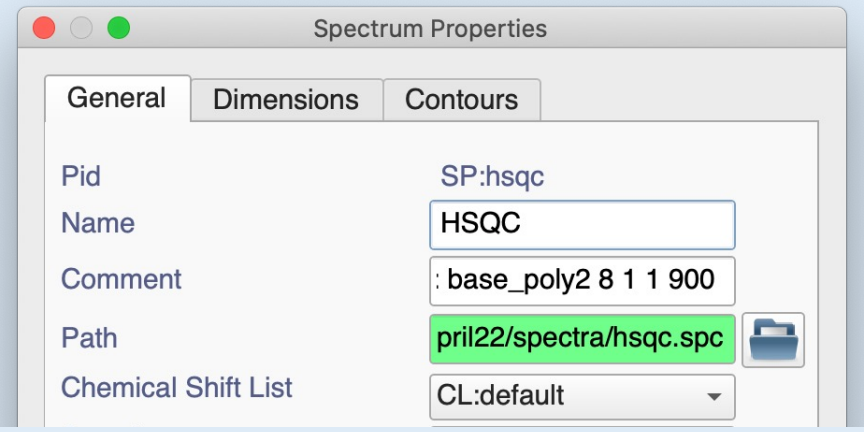
- Go to **Main Menu → View → Python Console**

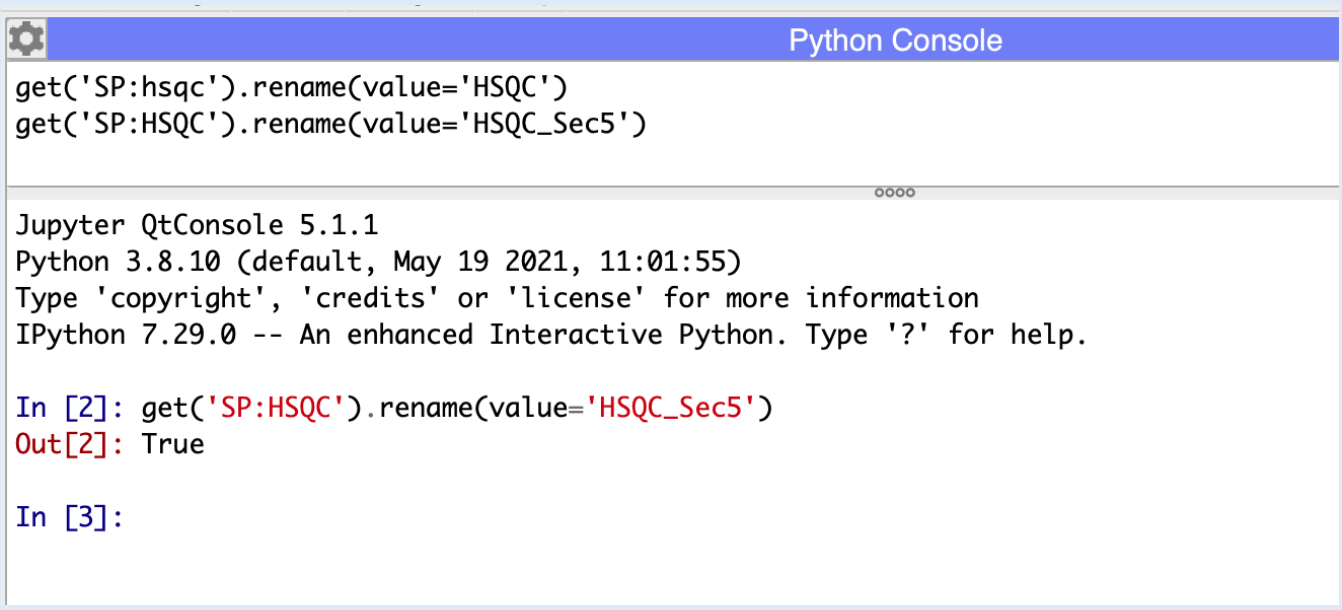
OR

- Use the shortcut **Space-Space**

The top half of the console will echo commands that you execute using the graphical user interface (GUI).
The lower half is where you can start typing commands.

2 Using the Python Console





2C Rename Spectrum in the GUI

- **Double-click** on the **hsqc** spectrum in the sidebar to bring up the **Spectrum Properties** dialog box.
- Change the name of the spectrum to **HSQC** and click **OK**.

In the top half of the Python Console you should see an echo of the command that renamed your spectrum:

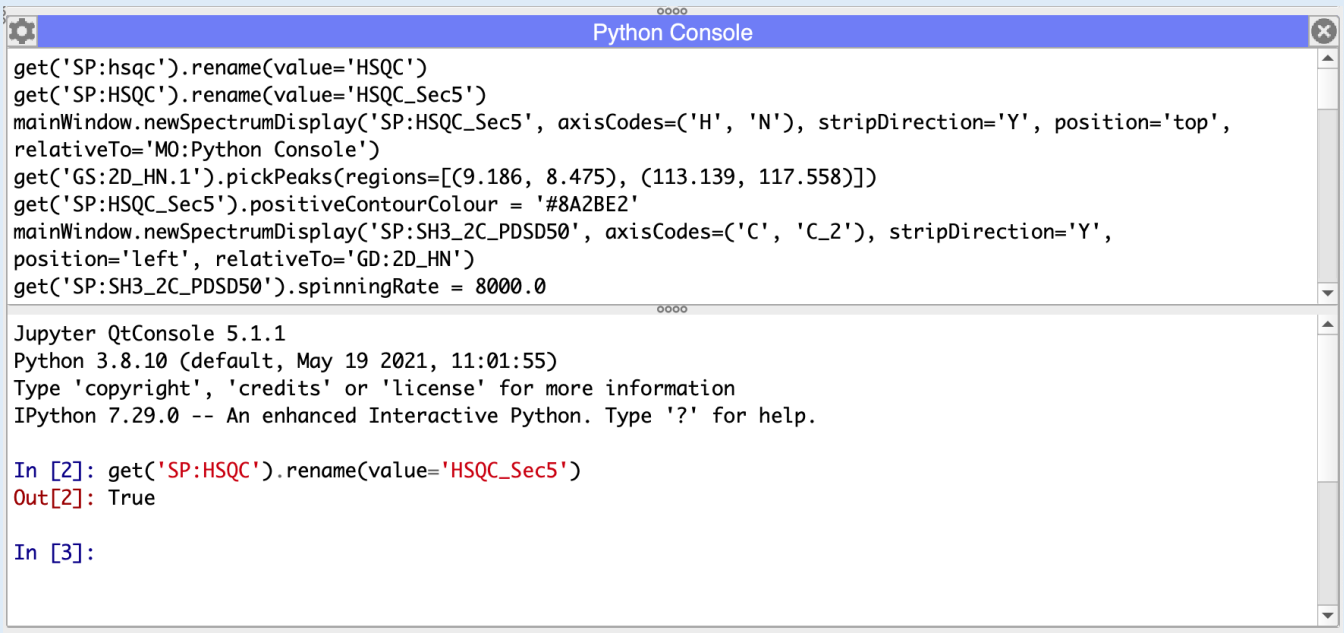
```
get('SP:hsqc').rename(value='HSQC')
```

2D Rename Spectrum in the Python Console

- Now have a go at renaming your spectrum in the lower part of the python console by typing

```
get('SP:HSQC').rename(value='HSQC_Sec5')
```

2 Using the Python Console



2E Try other commands

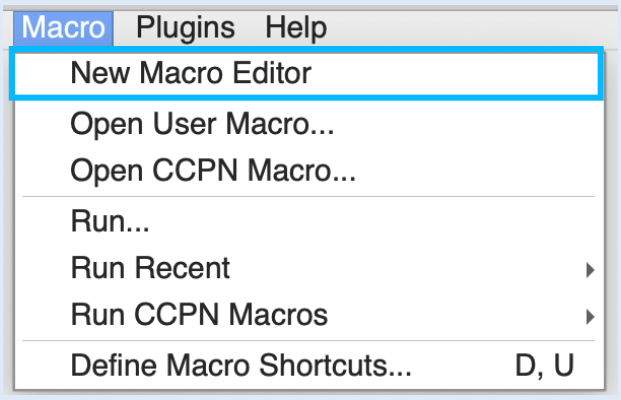
Try finding some other commands in the GUI and then executing them in the Python Console e.g.

- Peak pick a region in the HSQC_Sec5 spectrum with **Shift+Ctrl** (**Shift+Cmd** on a Mac) and **left-drag**.
- Change the spectrum contour colours (e.g. with shortcut **CO**).
- Double-click on the **sh3_2c_pdsd** in the sidebar to bring up the Spectrum Properties and in the **General** tab, set the **Spinning Rate** to **8000**. (You may afterwards like to **right-click** on the spectrum and choose **Customise** / **Show MAS Sidebands** to see the effect of chooseing different spinning rates.)
- Move a peak by selecting it and dragging it with the middle mouse button.
- Go to **Main Menu -> Assign -> Set up NmrResidues** and do this for the **HSQC_Sec5** spectrum
- Open the **Peak Assigner** with **AP** and Assign/Deassign some peaks.

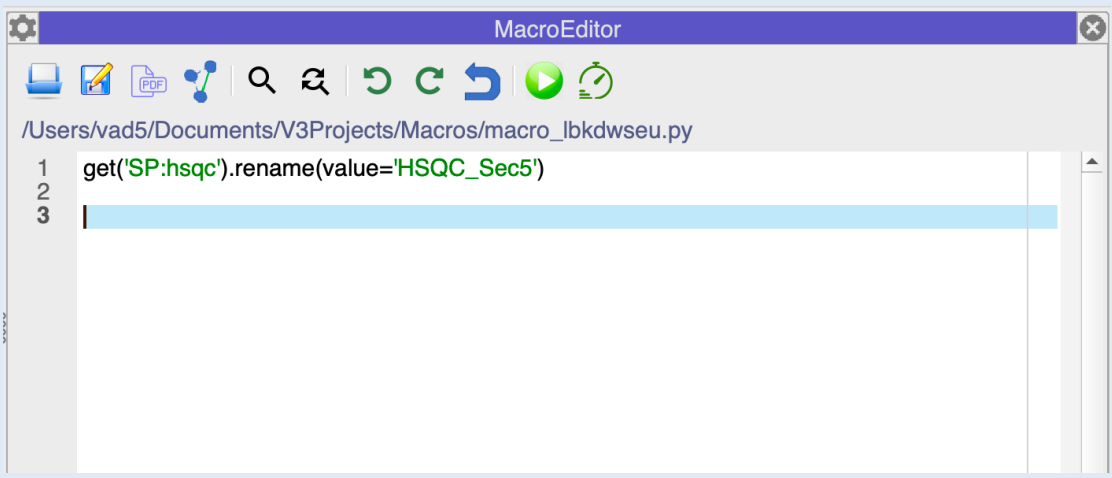
Notice that in some cases, a single operation on the GUI actually executes several commands on the Console.

Opening a new module is also echoed.

3 Using the Macro Editor



NM



3A Open Macro editor

- Go to **Main Menu → Macro → New Macro Editor**

OR

- use shortcut **NM**.

3B Write and Run Macro

- Type some of your commands from Section 2 into the Macro Editor, e.g.

  get('SP:HSQC').rename(value='Sec5_HSQC')

- Click on  to execute the macro

- Try executing several commands in one go, e.g.

  get('SP:hncacb').rename(value='HNCACB')

  get('SP:cbcaconh').rename(value='CBCACONH')

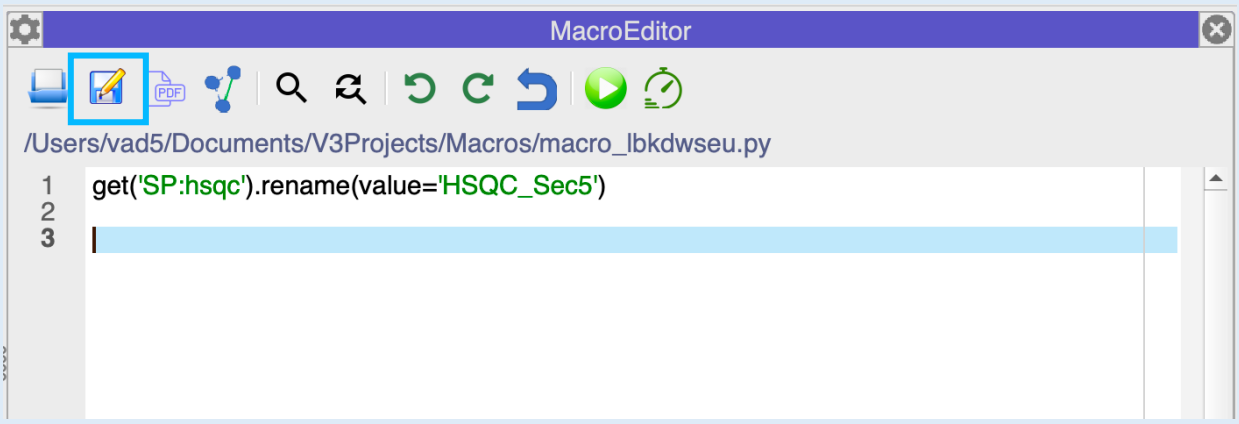
OR

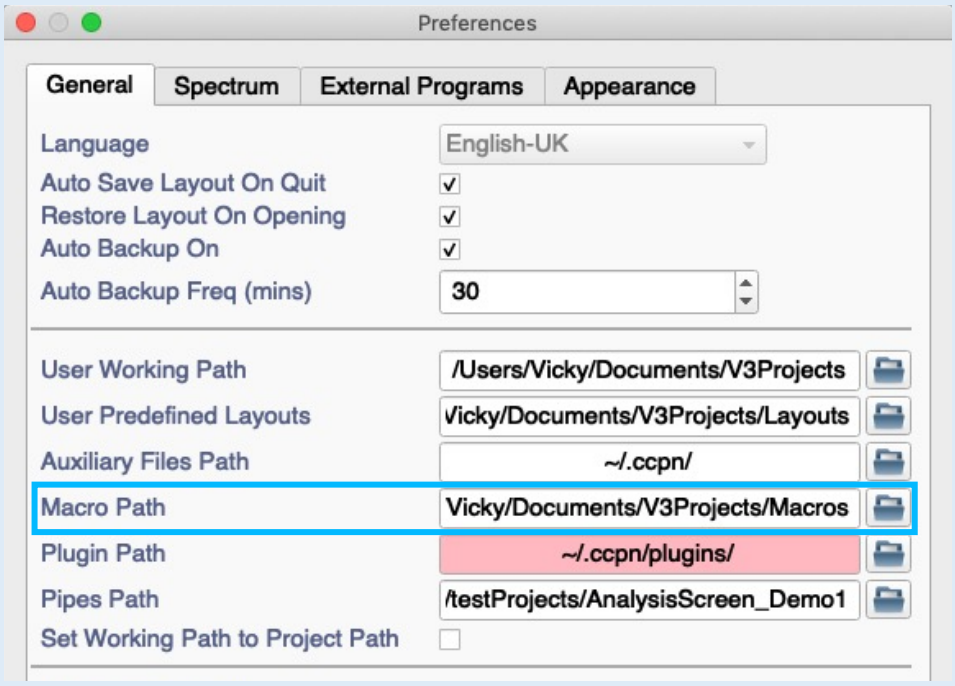
  get('SP:HSQC_Sec5').rename(value='HSQC')

  get('SP:HSQC').positiveContourColour = '#FFC800'

  get('GS:2D_HN.1').pickPeaks(regions=[(11.0, 5.0), (100.0, 135.0)])

3 Using the Macro Editor





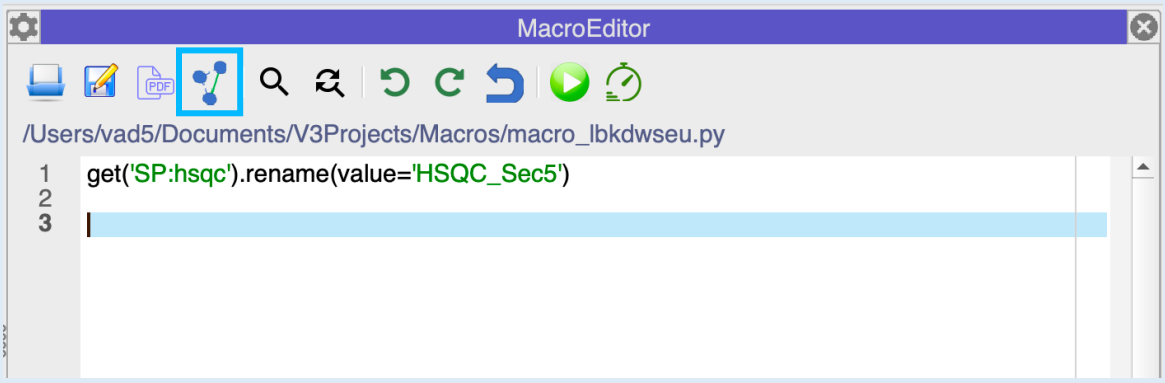
3C Save Macro

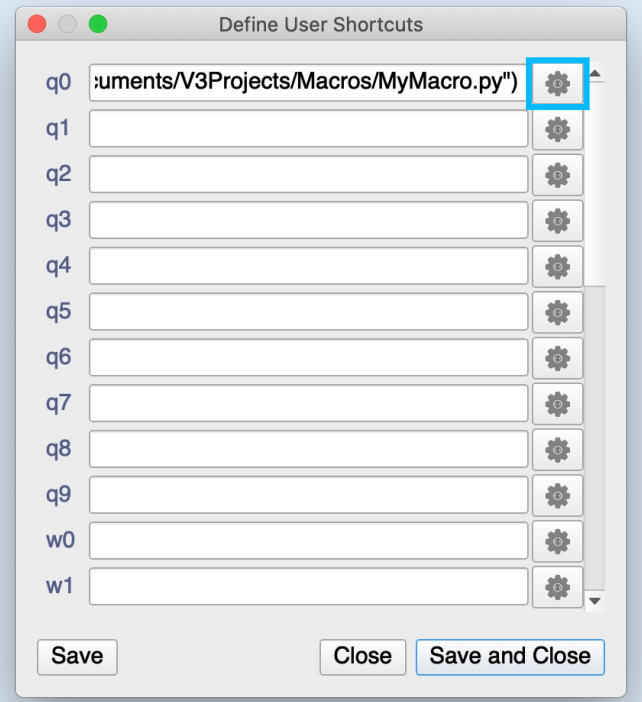
- Save one of your macros by clicking on the Save icon.

Note that you can set a default Macro directory in which to save all your macros in your User Preferences. To change this directory:

- Go to **Main Menu → Project → Preferences**…
- Change **Macro Path** to whichever directory you want to use instead.

3 Using the Macro Editor





3D Link macro to keyboard shortcut

- Click on in the button in the toolbar menu

OR

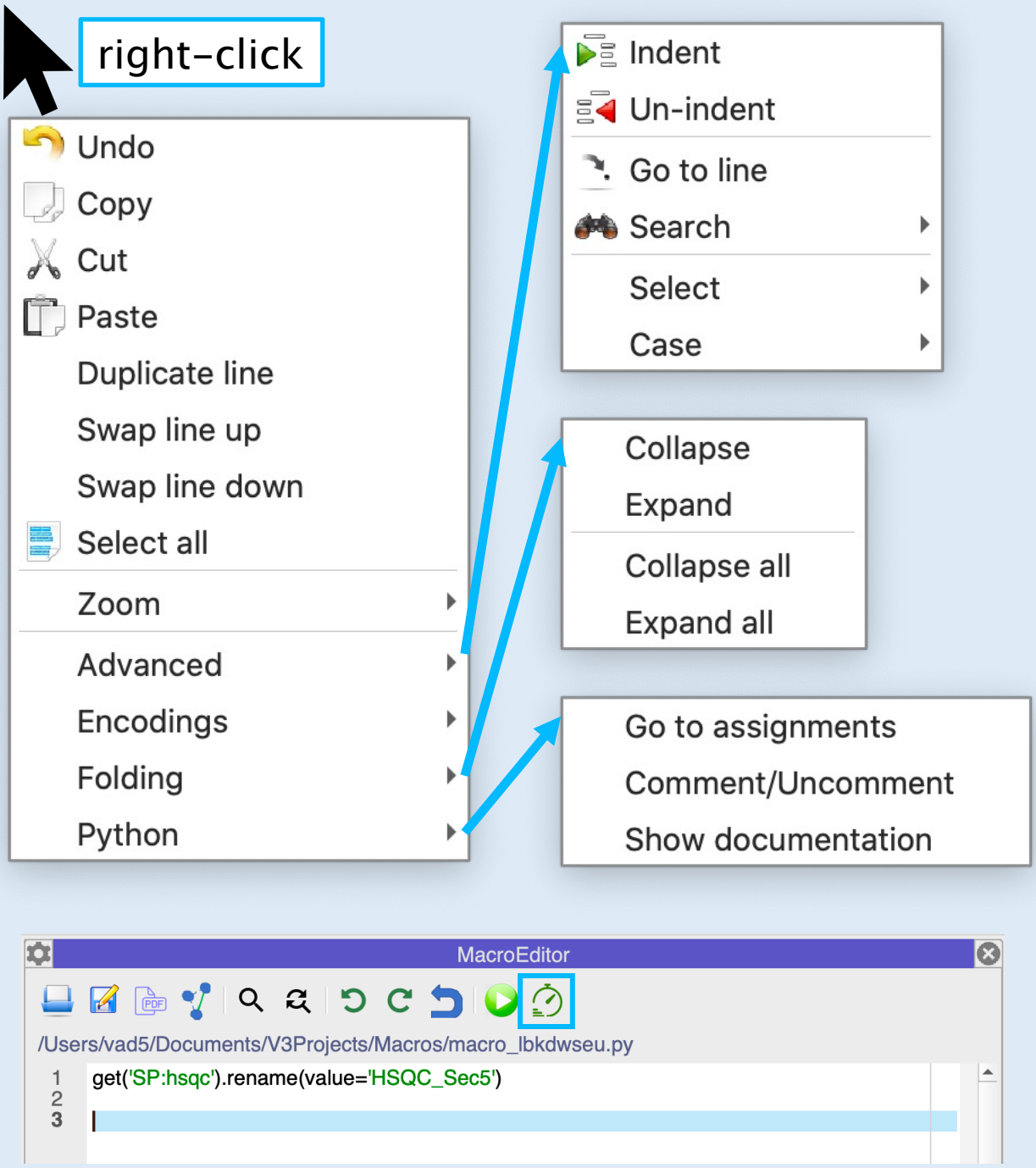
- Go to **Main Menu → Macro → Define Macro Shortcuts**…

OR

- Use the shortcut **DU**.

Select a shortcut code from the list and associate your macro with it by **clicking on the gear button** and selecting your macro in the file browser.

Using the Macro Editor

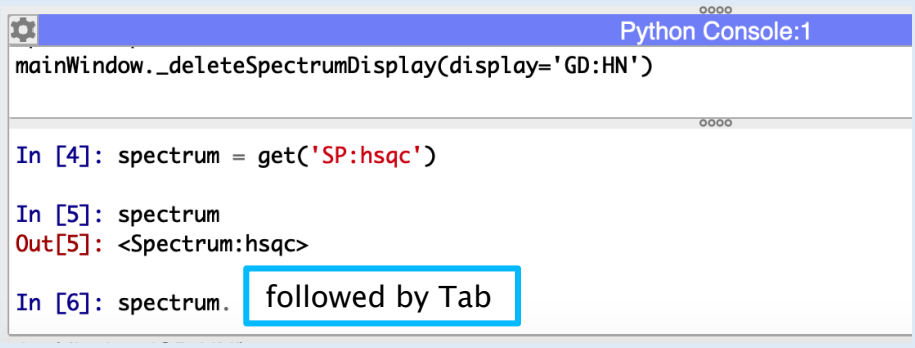


3E More Macro Editor Features

The **right-hand mouse menu** in the Macro Editor gives you access to a number of useful features, including being able to Comment/Uncomment, Indent/Un-indent or Collapse/Expand sections easily.

Advanced users may also find it useful to run more complicated macros using a profiler to help you identify areas for improvement. Rather than using the play button, run the macro with the stop watch icon: 

4 Finding Methods and Properties



4A Finding Methods and Properties via the Console

You can get a list of methods and properties belonging to an object in the Python Console.

- Following the example above, type

  ```
  spectrum = get('SP:GB1_hsqc')
  ```

  to assign the **SP:GB1_hsqc** object to the **spectrum** variable. (This is where **right-click** / **Copy Pid to Clipboard** can come in handy!)
- Typing

  ```
  spectrum
  ```

  should echo the object (see above) – a useful way to check for typos.
- Typing

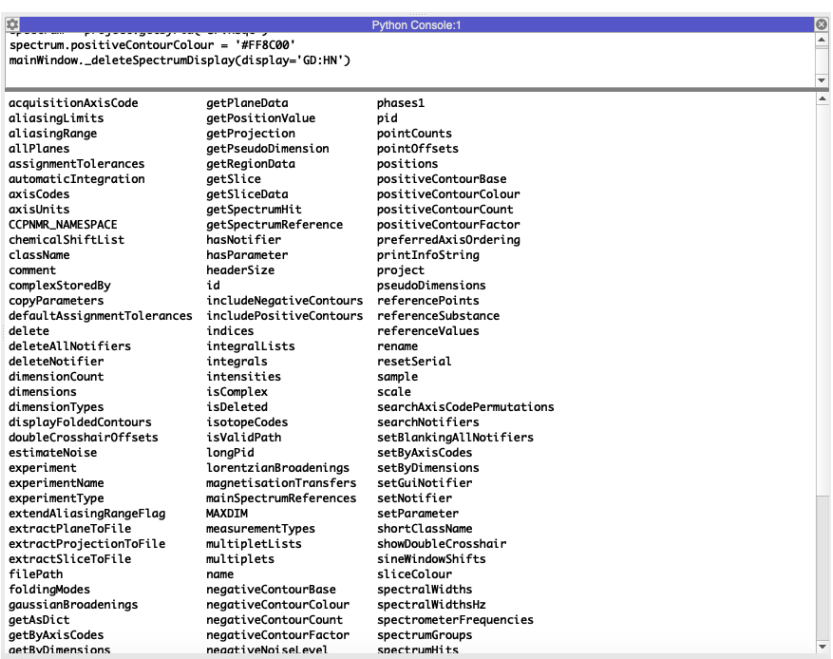
  ```
  spectrum.
  ```

  followed by **Tab** will give you a list of the methods and properties available to a **spectrum** object.
- Type **Esc** to remove the list again.

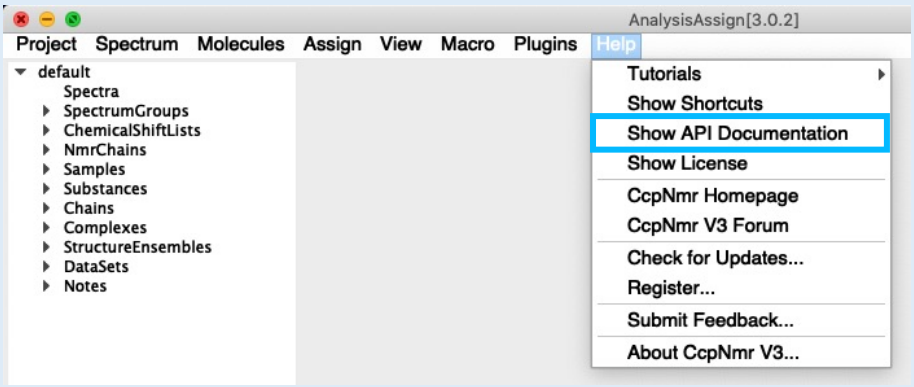
You can also type

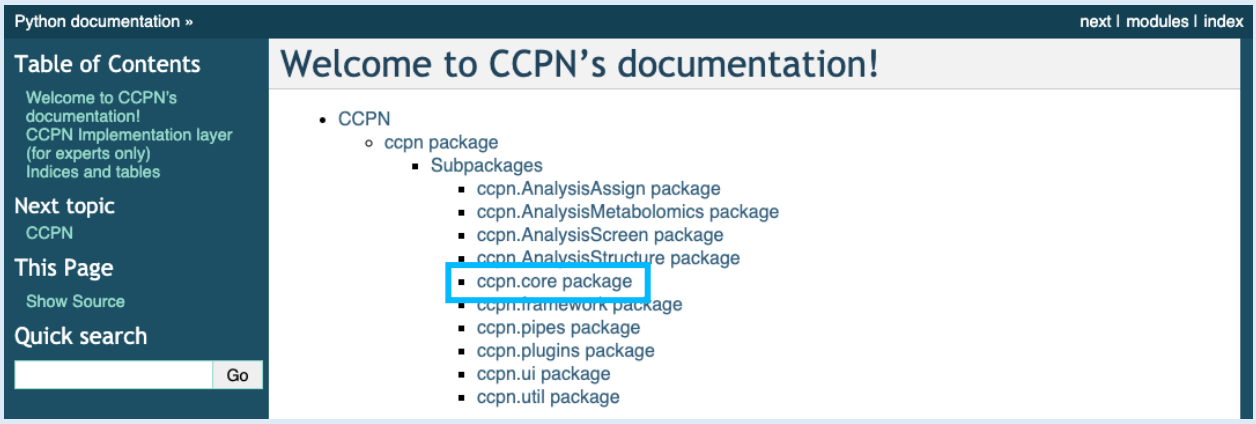
```
spectrum.p
```

followed by **Tab** in order to see all methods and properties beginning with **p** etc.



4 Finding Methods and Properties





4B Finding Methods and Properties via the API Documentation

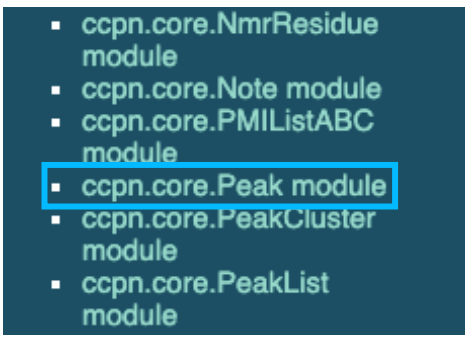
- Go to **Main Menu → Help → Show API Documentation**

to bring up the API Documentation.

(Go to **Main Menu → Project → Preferences** and select **Use Native Web Browser** to view the documentation in your usual web browser, or deselect to to view it in a module within the program.)

- Click on **ccpn.core package**.

The left-hand menu gives you a list of all the data types/classes. To view methods and properties associated with **Peaks**, for example, click on **ccpn.core.Peak module**.



Methods are then shown in bold with the option of viewing the source code by clicking on **[source]**:

addAssignment(*value: Sequence[str | NmrAtom]*) [source]

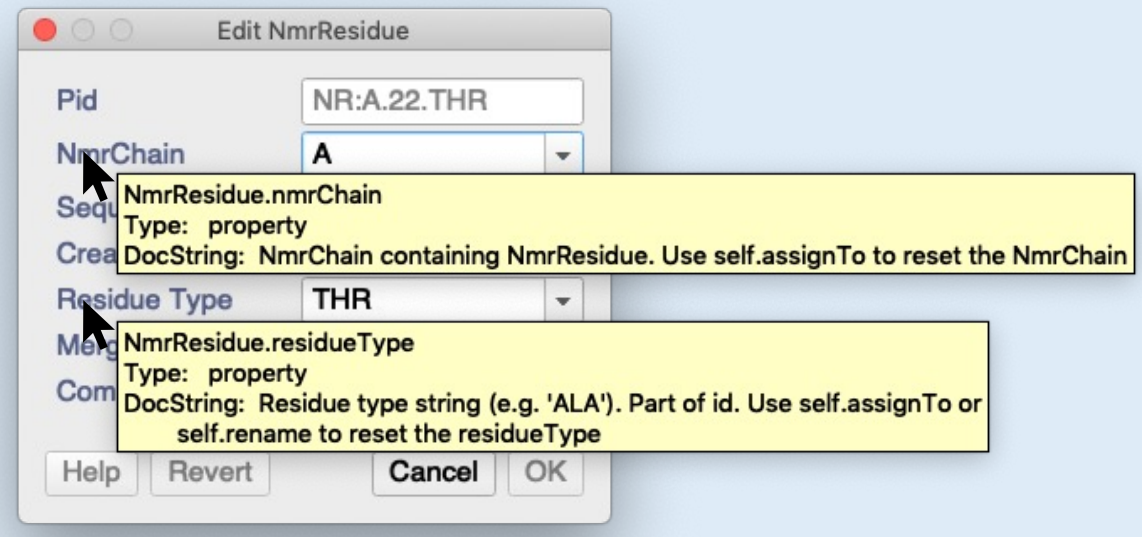
Add a peak assignment - a list of one NmrAtom or Pid for each dimension

Properties are are marked as properties:

property **aliasing**

- *Tuple[float=None, …], mutable* - Aliasing for the peak in each dimension. Defined as integer number of spectralWidths added or subtracted along each dimension

4 Finding Methods and Properties

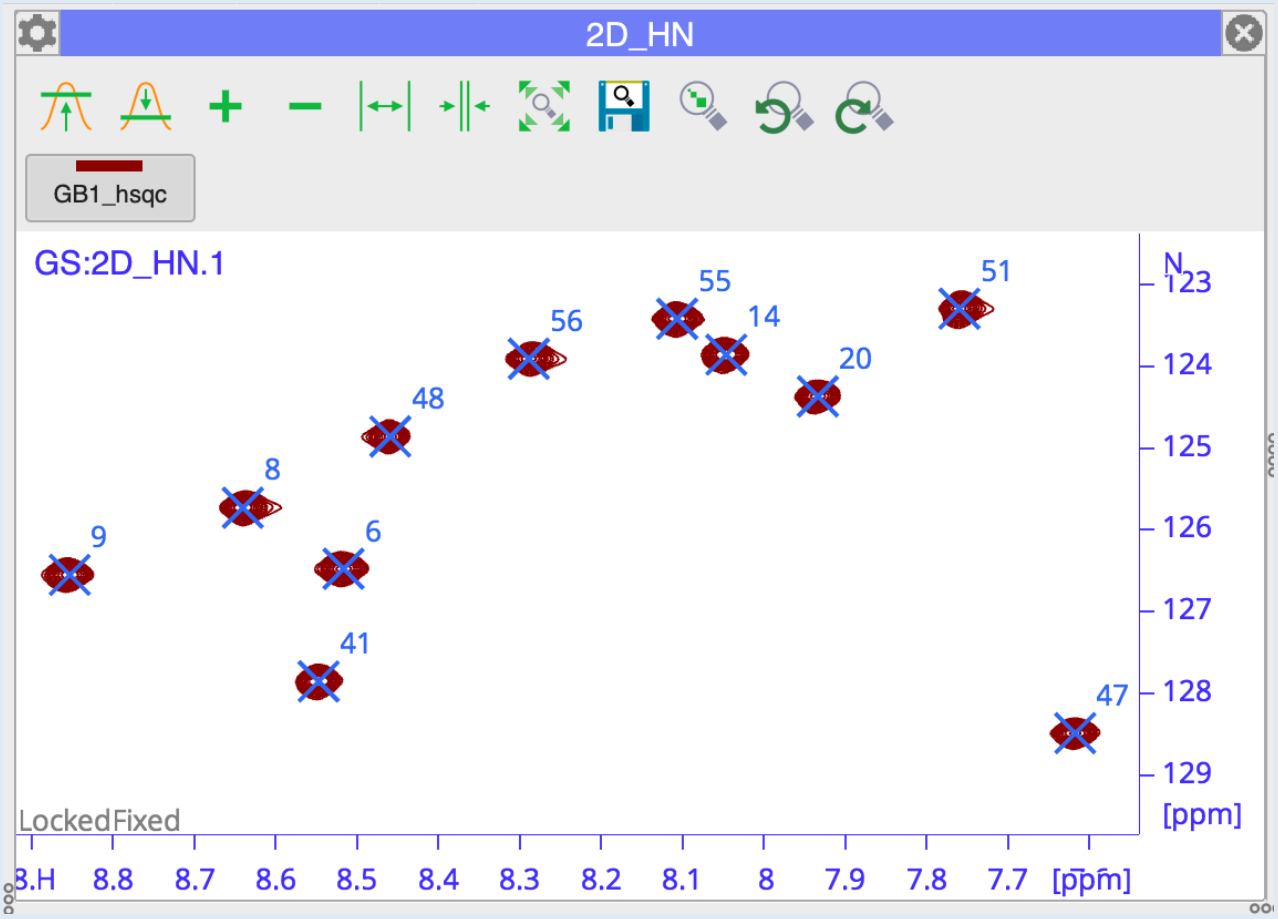


4C Finding Properties in pop-ups

- **Double-click** on an object in the sidebar to bring up a pop-up that will allow you to edit the object.
- **Move the mouse** over the descriptions on the left. Those which are properties of the object will bring up a tooltip after a few seconds which shows you the property name and a brief description.

The pop-ups do not contain an exhaustive list of all object properties, but it can be a quick way to find a property and some related methods.

4 Finding Methods and Properties



4D Exercises

1. Write a short macro to change the symbol and peak label colours of to a blue colour (e.g. #3A6BEC).
2. Get a peak's position in ppm and in points. (hint: use **`print()`** to show your result)
3. Find the spectra associated with the 'default' chemical shift list.
4. Renumber the NC:GB1 NmrChain, increasing the sequence number by 2.
5. Count the number of peaks in the PL:GB1_hsqc.2 peak list. (hint: **`len()`** will measure the length of a list or tuple).

Possible answers are in the **CcpnTutorialDataMacroWritingApril22/macros** folder:

4D.1.changePeakListColours.py

4D.2.printPeakPositions.py

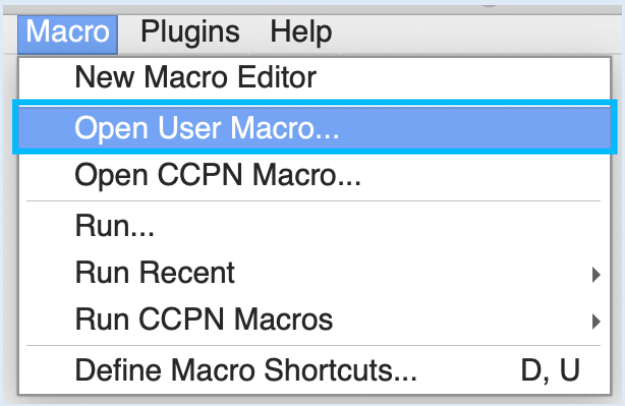
4D.3.printCSLSpectra.py

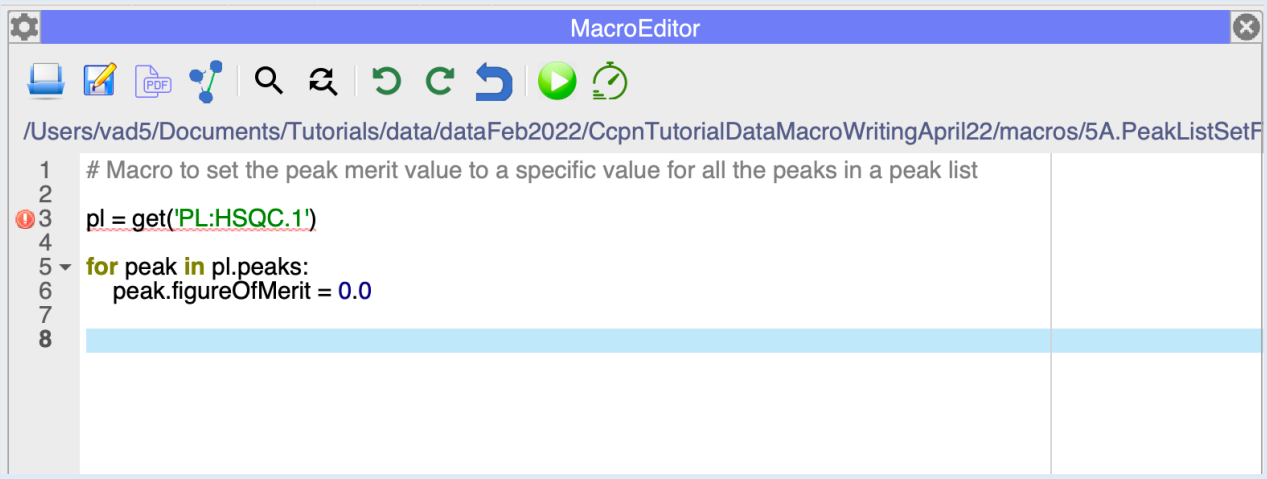
4D.4.renumberNmrChain.py

4D.5.countPeaks.py

5 Loops and conditionals

Often you will want to manipulate not just one item of data, but several. This section will show you how you can easily loop through items of data.





5A Looping through Peaks in a Peak List

- Go to **Main Menu → Macro → Open User Macro**... and open the **5A.peakListSetFigureOfMerit.py** macro from the **CcpnTutorialDataMacroWritingApril22/macros** directory.

This macro will loop through all the peaks in a peak list and set the peak merit value to 0.0. This might be useful if you have a peak list whose peaks you don't want to contribute to the chemical shift list.

Comments:

Line 3 sets the peak list that will be used via its **PID**. Change this if you want to use a different peak list.

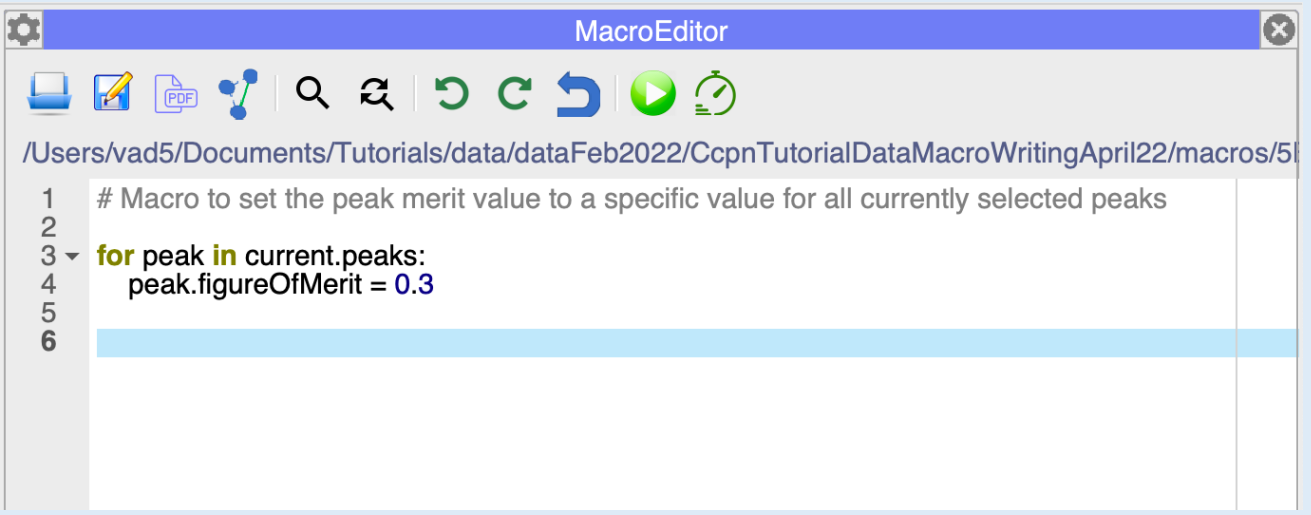
Line 5 loops through the peaks in the peak lists using **pl.peaks**. The **PeakList** property **peaks** contains all the **peak** objects in that peak list.

All data types / classes that have child classes, have such a property, e.g. all NmrAtoms in an NmrResidue are given by the **nmrAtoms** property, all PeakLists in a Spectrum are given by the Spectrum property **peakLists** etc.

Line 6 sets the new figure of merit to 0.

5 Loops and conditionals

In order to loop through currently selected items, you can use current.



5B Using 'Current' to loop through selected peaks

- Go to **Main Menu → Macro → Open**... and open the **5B.currentPeaksSetPeakMerit.py** macro from the **CcpnTutorialDataMacroWritingApril22/macros** directory.

This macro is similar to the one in **Section 5A**, except that rather than looping through all the peaks in one peak list, it loops through all the currently selected peaks.

You can use **current** to loop through many currently selected objects such as peaks, peakLists, nmrAtoms/Residues/Chains, chemicalShifts, chemicalShiftLists, restraints, samples, substances, spectrumGroups etc. (see next page for a full list).

You also have access to some GUI (graphical user interface) elements, including cursorPosition, guiTable and strip.

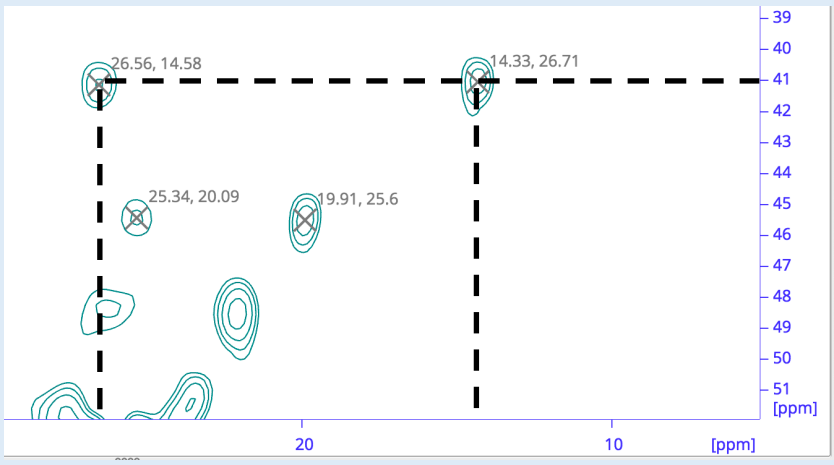
Spectrum is not included, because you can't select a spectrum. Instead, use **current.strip.spectra** as a way to access a selected spectrum or set of spectra.

For most items both the plural and singular exist, i.e. **peaks** and **peak**. **Current.peaks** will give you all the currently selected peaks; **current.peak** will only give you the most recently selected peak, even if other peaks have been selected as well.

Objects available in 'Current'

axisCode
chain / chains
chemicalShift / chemicalShifts
chemicalShiftList / chemicalShiftLists
collection / collections
cursorPosition
dataTable / dataTables
guiTable
integral / integrals
macroFile / macroFiles
multiplet / multiplets
nmrAtom / nmrAtoms
nmrChain / nmrChains
nmrResidue / nmrResidues
pcaComponent / pcaComponents (AnalysisScreen and AnalysisMetabolomics)
peak / peaks
pid
position / positions
project
residue / residues
restraint / restraints
sample / samples
spectrumGroup / spectrumGroups
spectrumHit (AnalysisScreen)
strip
substance / substances
violationTable
violationTables

5 Loops and conditionals



y = 14.4 + 26.6
= 41.0

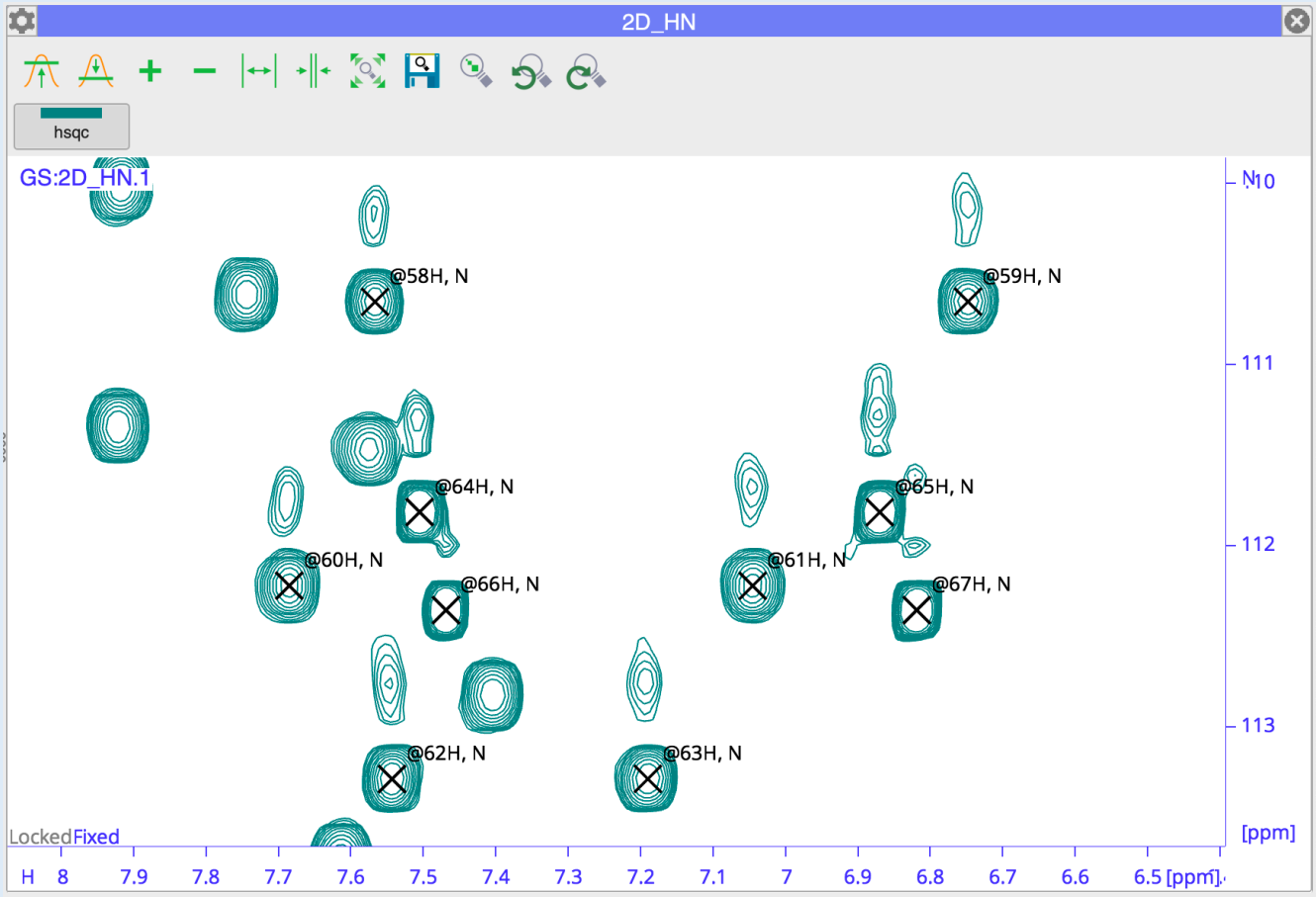
x = ~26.6 x = ~14.4

5C Excercises

1. Add ‘new_’ to start of each spectrum name (hint: use f-strings or join() to do the actual addition of the prefix)
2. Add a comment (such as 'noise?') to all currently selected peaks.
3. Deconvolute the chemical shifts in a DQ spectrum: the **SP:yada_postc7** spectrum is a double quantum (DQ) spectrum in which each peak position reflects two chemical shifts (CS1 and CS2) at position x = CS1 and y = CS1 + CS2 (see above). Pick some peaks in this spectrum (note they come in horizontal pairs!) and then write a macro to deconvolue them and place them in the peak Annotation. At the end you can go to the Spectrum Settings and select **Annotation** to display the chemical shifts.

Suggested answers are in the **macros** directory.

5 Finding Methods and Properties



5D Fetch

1. **SP:hsqc** (or whatever you have renamed it to!) contains a set of peaks which have been set up with NmrAtoms using the **Assign/Set up NmrAtoms** feature. This assumes that all atom names will be **H** and **N**. But of course some peaks will belong to Asn/Gln side chains and therefore be **ND2** and **HD21/22** or **NE2** and **HE21/22** atoms.
   Write a macro which allows the user to select a pair of Asn/Gln side-chain peaks and then automatically changes the NmrAtom names to **ND2/NE2** and **HD/E21** or **HD/E22** and the residue type to **ASN/GLN**.

Our example solution macro includes a method called **fetchNmrAtom**. You will find that many objects have a **fetch** method associated with them. **Fetch** methods will always look to see if the specified object already exists and if it does, it will **get** it. If it doesn't already exist, it will **create** it. It is avery useful method to use when you want to use an object and can't be sure whether it exists already or not. It means you will neither accidentially try and **get** an object that doesn't yet exist or try and **create** an object that does already exist.

5 Loops and conditionals

```
if x == 1.0:
    do something
elif 1.0 < x <= 10.0:
    do something different
else:
    do something different again

if x != 'this_string':

if peak.lineWidth is None:

if len(project.spectra) >= 1:

if project.spectra:
```

5E Introducing conditionals

Above is a reminder of some of the conditionals that you can use in python and you might find useful.

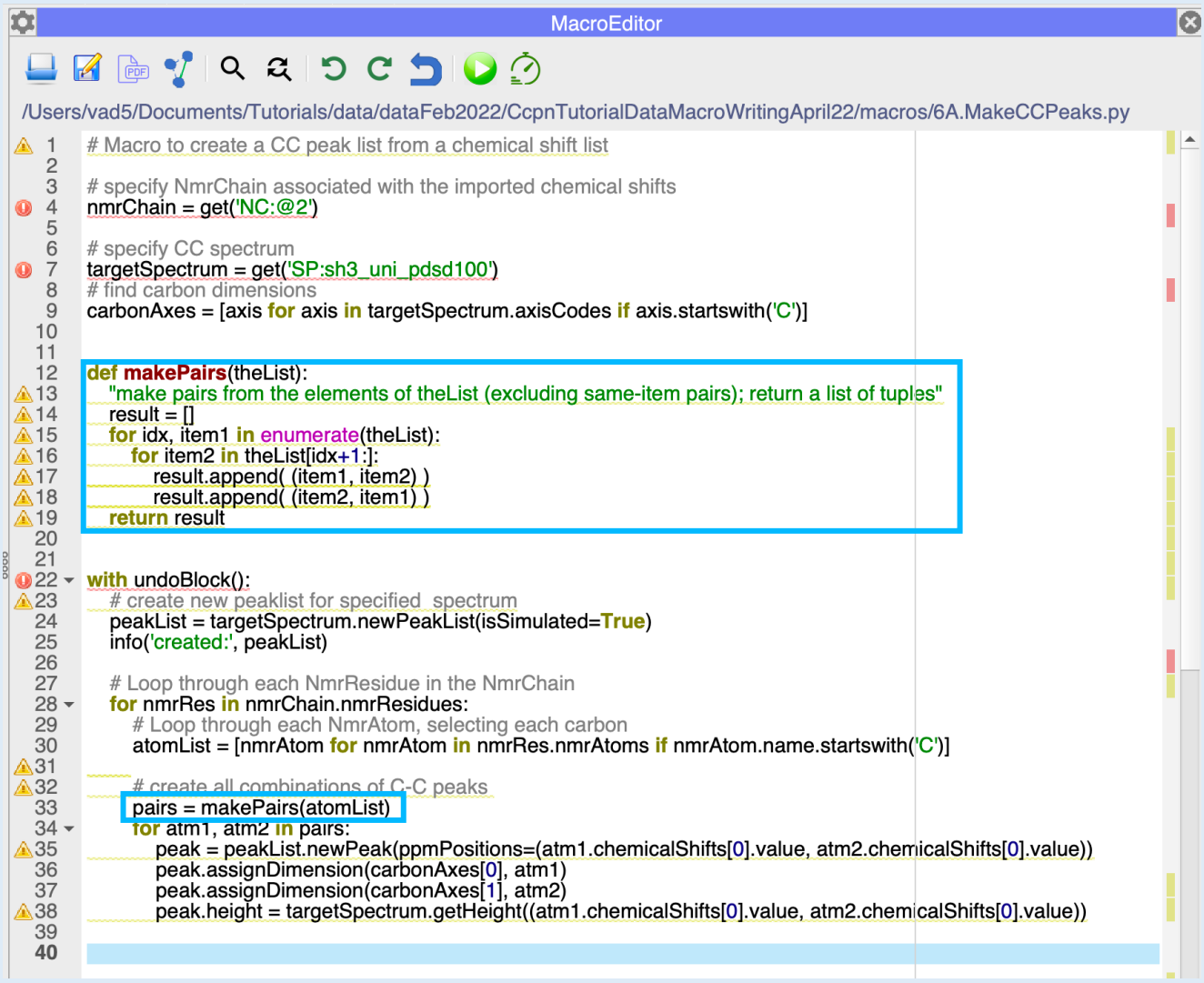
Note that **None** means something is undefined. You will sometimes see the word **None** in tables, e.g. the lineWidth of a peak could be **None**. Remember that **None** is not the same as **0.0**, although some routines will treat them the same (**if not peak.lineWidth:** will find line widths that are None *and* 0.0). Try to be as precise as you can in your coding!

5F Excercises

Write macros using loops and conditionals to the do the following

1. Change the 'Hn' NmrAtom names in the NC:GB1 NmrChain to 'H'.
2. Delete all the NmrAtoms in the NC:GB1 NmrChain that do not have any chemical shifts associated with them.
3. Delete all unassigned peaks in the **PL:GB1_hsqc.2** peak list.
4. Delete all diagonal peaks in the **PL:sh3_2c_pdsd50.1** peak list. (You will need to decide what kind of tolerance to work with.)
5. Move currently selected peaks in the **PL:sh3_2c_pdsd50.1** peak list to its sister peak list **PL:sh3_2c_pdsd50.2**.
6. Merge the -1 NmrAtoms in the NC:A nmrChain into the NmrAtom of the previous residue.

6 Subroutines / Functions



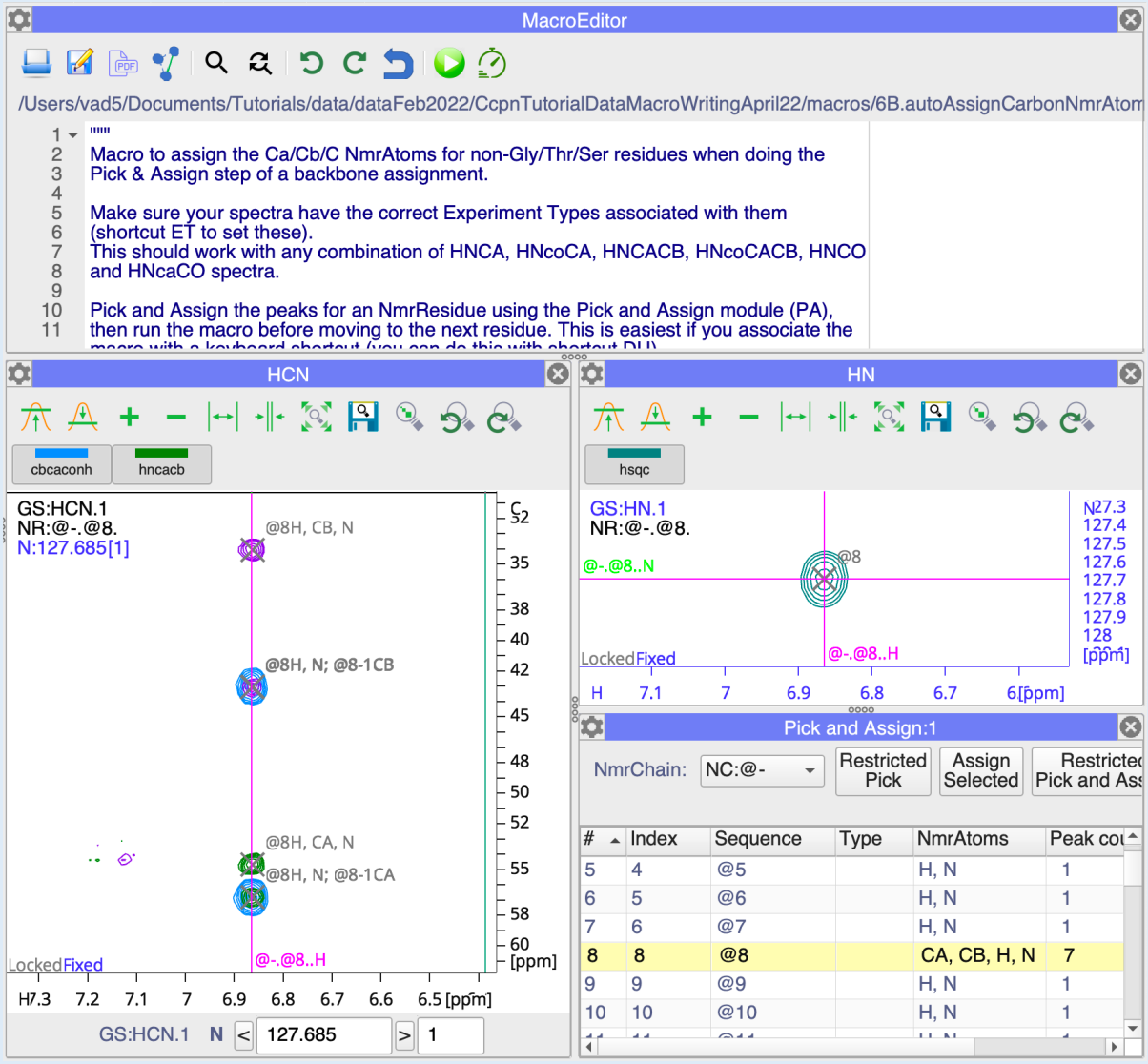
6A Subroutine/Function Basics

- Go to **Main Menu → Macro → Open**... and open the **6A.MakeCCPeaks.py** macro in the **macros** directory.
  This macro will create intra-residue peaks for a ^{13}C–^{13}C correlation spectrum and contains a subroutine called **makePairs** (boxed in image above).

  The **def** command (short for **define**) marks the beginning of the function and the remainder is indented.
  makePairs is the function name which is used lower down to call it.
  theList is (in this case) the only input parameter used by the function and when the function is called, an appropriate parameter must be specified. Use **()** for no input parameters and **(theList, anotherList, theTuple)** for several.
  return marks the end of the function with **result** (in this case a list) being passed back to the main program.

  Using subroutines or functions is good programming practice and you should try to use them whenever you can, especially to avoid code duplication.

6 Subroutines / Functions



6B Subroutine/Function example

This is another example of a macro which uses a function to avoid code duplication.

- Open the **CcpnTutorialDataMacroWritingApril22/Sec5Assignment.ccpn** project.
- Go to **Main Menu → Macro → Open User Macro**... and open the **6B.autoAssignCarbonNmrAtoms** macro in the macro directory.
- Go to the **Pick and Assign** settings to set your Target display as **GD:HCN**.
- **Double-click** on an NmrResidue in the **Pick and Assign** table (e.g. @8). If the residue pattern does not include Gly/Thr/Ser, then the macro will automatically assign the Carbon NmrAtoms for you. Run the macro in the editor or assign it to a keyboard shortcut.

7 Worked Example

```
"""
This Macro illustrates how to work with spectral data and spectral parameters.
It creates a series of nD spectra from a pseudo-nD spectrum, collated in a new
spectrumGroup.

"""

# The pseudo3D spectrum
spectrum = get('SP:Bruker-pseudo3D-1')


def splitPseudo3DSpectrumIntoPlanes(spectrum):
    # we first establish what the "Time" dimension is
    # getByAxisCodes returns a list, so we take first element
    timeDimension = spectrum.getByAxisCodes('dimensions', ['Time'])[0]

    # Find the number of points along the Time dimension
    # dim's and positions are 1-based; python lists/tuples are zero-based
    timeDimensionSize = spectrum.pointCounts[timeDimension-1]

    # get the frequency dimensions; ie. all dimensions that are not Time dimension(s)
    # Python's list comprehensions are a powerful way of doing this
    freqDims = [dim for dim in spectrum.dimensions if dim != timeDimension]
    # and the corresponding axis codes using build-in functionality of the Spectrum class
    freqAxisCodes = spectrum.getByDimensions('axisCodes', freqDims)

    # Anything could define the series values of a spectrumGroup
    # Assume that the series values are defined by the spectralWidth/dwellTime
    # This is likely incorrect, but can be corrected later if need be.
    seriesValue = 0.0
    seriesIncrement = 1.0 / spectrum.spectralWidths[timeDimension-1]
    seriesUnits = 'ms'

    # For now: we need this to silence some of the output
    with notificationEchoBlocking():
        # For now: we want all of this to be one "undo" operation
        with undoBlock():

            # Create a new spectrumGroup to collate the newly created spectra
            spectrumGroup = project.newSpectrumGroup(name=spectrum.name, seriesUnits=seriesUnits)

            position = [1]*spectrum.dimensionCount  # dims and positions are 1-based

            # loop over the points in the time dimension
            for timePoint in range(timeDimensionSize):

                # set the position of the plane we are now doing
                # dims and positions are 1-based; Python is zero-based
                position[timeDimension-1] = timePoint + 1

                info(f'==> extracting {freqAxisCodes} plane at {position}' )

                sp = spectrum.extractPlaneToFile(axisCodes = freqAxisCodes, position = position)
                spectrumGroup.addSpectrum(sp, seriesValue)

                seriesValue += seriesIncrement


# Check if we have a valid spectrum for the macro to function
if not 'Time' in spectrum.dimensionTypes:
    warning('This macro only works for pseudo-nD spectra; no time axis found.')
else:
    splitPseudo3DSpectrumIntoPlanes(spectrum)
```

most of macro is contained in this function

find a dimension from its AxisCode

silence terminal messages

wrap a set of operations into a single Undo operation

output an information message to the terminal

write out the NMR data

output a warning to the terminal

The actual macro consists of just these few lines at the bottom which include a test to see if the input data was appropriate or not

7A Pseudo 3D to SpectrumGroup

The **7A.pseudo3dToSpectrumGroup.py** macro will take a Pseudo 3D spectrum and split it up into individual planes which are written out as **.ndf5** spectra and placed into a new SpectrumGroup. This macro illustrates some useful methods including how to extract raw data from a spectrum and write it into a new file.

- Try it out using the **Bruker-pseudo3D.zip** spectrum in the **spectra** directory.

External modules included in the V3.1 environment

Advanced users who are familiar with these packages, can include these in their macros if they wish. We've highlighte some of the most popular ones.

alabaster 0.7.12
appnope 0.1.2
asn1crypto 1.4.0
asttokens 2.0.5
babel 2.9.1
backcall 0.2.0
backports 1.1
backports.shutil_get_terminal_size 1.0.0
biopython 1.78
blas 1.0
bottleneck 1.3.2
brotli 1.0.9
brotlipy 0.7.0
bzip2 1.0.8
c-ares 1.18.1
ca-certificates 2021.10.26
cairo 1.16.0
certifi 2021.10.8
cffi 1.15.0
chardet 4.0.0
charset-normalizer 2.0.4
colorama 0.4.4
cryptography 36.0.0
curl 7.80.0
cycler 0.11.0
cython 0.29.25
dbus 1.13.18
debugpy 1.5.1
decorator 5.1.0
docutils 0.17.1
entrypoints 0.3
et_xmlfile 1.1.0
executing 0.8.2
expat 2.4.1
fontconfig 2.13.1
fonttools 4.25.0
freetype 2.11.0
fribidi 1.0.10
get_terminal_size 1.0.0
gettext 0.21.0
giflib 5.2.1
git 2.34.1
glib 2.68.2
graphite2 1.3.14
h5py 3.5.0
harfbuzz 2.8.1
hdf5 1.10.6
icecream 2.1.1
icu 68.1
idna 3.3
imageio 2.9.0
imagesize 1.3.0
intel-openmp 2022.0.0
ipykernel 6.4.1
ipython 7.29.0
ipython_genutils 0.2.0
jbig 2.1
jdcal 1.4.1
jedi 0.17.2
jinja2 3.0.2
joblib 1.1.0
jpeg 9d
jupyter_client 7.1.0
jupyter_core 4.9.1
kiwisolver 1.3.1
krb5 1.19.2
lcms2 2.12
libclang 11.1.0
libcurl 7.80.0
libcxx 12.0.0
libcxxabi 4.0.1
libedit 3.1.20210910
libev 4.33
libffi 3.3
libgfortran 3.0.1
libglib 2.68.2
libiconv 1.16
libllvm11 11.1.0
libnghttp2 1.46.0
libopenblas 0.3.13
libpng 1.6.37
libpq 13.3
libsodium 1.0.18
libssh2 1.9.0
libtiff 4.2.0
libwebp 1.2.0
libwebp-base 1.2.0
libxml2 2.9.12
libxslt 1.1.33
llvm-openmp 12.0.0
llvmlite 0.37.0
lz4-c 1.9.3
markupsafe 2.0.1
matplotlib 3.5.0
matplotlib-base 3.5.0
matplotlib-inline 0.1.2
memory_profiler 0.58.0
mkl 2022.0.0
munkres 1.1.4
mysql-common 8.0.25
mysql-libs 8.0.25
ncurses 6.3
nest-asyncio 1.5.1
nomkl 3.0
nose 1.3.7
nspr 4.32
nss 3.69
numba 0.54.1
numexpr 2.8.1
numpy 1.20.3
numpy-base 1.20.3

External modules included in the V3.1 environment

continued

olefile 0.46
openbabel 3.1.1
openblas 0.3.13
openblas-devel 0.3.13
openpyxl 3.0.9
openssl 1.1.1m
packaging 21.3
pandas 1.3.5
pango 1.45.3
parso 0.7.0
path 16.2.0
path.py 12.5.0
pcre 8.45
pcre2 10.37
perl 5.26.2
pexpect 4.8.0
pickleshare 0.7.5
pillow 8.4.0
pip 21.2.4
pixman 0.40.0
prompt-toolkit 3.0.20
prompt_toolkit 3.0.20
psutil 5.8.0
ptyprocess 0.7.0
pycparser 2.21
pygments 2.10.0
pyopenssl 21.0.0
pyparsing 3.0.4
pyqt 5.12.3
pyqt-impl 5.12.3
pyqt5-sip 4.19.18
pyqtchart 5.12
pyqtgraph 0.11.0
pyqtwebengine 5.12.1
pysocks 1.7.1
python 3.8.10
python-dateutil 2.8.2
python-pptx 0.6.21
python_abi 3.8
pytz 2021.3
pyyaml 6.0
pyzmq 22.3.0
qt 5.12.9
qtconsole 5.1.1
qtpy 1.10.0
readline 8.1.2
reportlab 3.5.67
requests 2.27.1
scikit-learn 1.0.2
scipy 1.7.3
seaborn 0.11.2
setuptools 58.0.4
simplegeneric 0.8.1
sip 4.19.25
six 1.16.0
snowballstemmer 2.2.0
sphinx 4.2.0
sphinx_rtd_theme 0.4.3
sphinxcontrib-applehelp 1.0.2
sphinxcontrib-devhelp 1.0.2
sphinxcontrib-htmlhelp 2.0.0
sphinxcontrib-jsmath 1.0.1
sphinxcontrib-qthelp 1.0.3
sphinxcontrib-serializinghtml 1.1.5
sqlite 3.37.0
tabulate 0.8.9
tbb 2021.5.0
threadpoolctl 2.2.0
tk 8.6.11
tornado 6.1
tqdm 4.62.3
traitlets 5.1.1
urllib3 1.26.7
wcwidth 0.2.5
wheel 0.37.1
xlrd 2.0.1
xlsxwriter 3.0.2
xz 5.2.5
yaml 0.2.5
zeromq 4.3.4
zlib 1.2.11
zstd 1.4.9
asteval 0.9.26
docx 0.2.4
future 0.18.2
hjson 3.0.2
lmfit 1.0.3
lxml 4.7.1
nmrglue 0.8
pycodestyle 2.8.0
pyflakes 2.4.0
pynmrstar 3.3.0
pyopengl 3.1.5
pyopengl-accelerate 3.1.5
pyqode-core 2.12.1
pyqode-python 2.12.1
pyqode-qt 2.10.0
uncertainties 3.1.6
pyqode-qt

Advanced Python users can go on to include GUI elements, including messages, selection boxes or plots. Please ask the CCPN team for more information or examples of this.

Contact Us

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Suggestions and comments:
support@ccpn.ac.uk

Issues and bug reports:
https://forum.ccpn.ac.uk/

Cite Us

Skinner, S. P. et al. CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. J. Biomol. NMR 66, (2016)