Starting Xipp on Linux
from a terminal window

xipp

Ensure that ~/Xipp is on your path or create an alias.
No args to start XippPanel in current directory.
Click 'Studies' to show all Studies in Directory.
Click 'New' to create a new Study, Molecule,
Assign Table or Structure.
Click Button next to Path to change current directory.

xipp HprE1_96
xipp dCBCACONH%03d.DAT
xipp HNCACB

Name of NMRPipe NMR Exp such as:
2D 15N HSQC,
3D CBCA(CO)NH stored in separate 2D planes,
3D HNCACB in a single file
This form will only show the single Exp and does not start XippPanel.

xipp backbone.xipp

Directly start Study backbone.xipp without starting XippPanel

xipp startXipp.py

Start Xipp from Python file by creating and initializing DataServer and GUI Objects.
New Java Objects are first implemented here and in Python library before XippPanel.

Do not start Xipp from a File Browser such as nautilus since Linux does a poor job identifying file type and associating correct application. If really want to do this you must associate the extension .xipp with xipp which is installed at ~/Xipp/xipp by default.

Under Linux a XippPanel is only started when xipp starts with no arguments.

xippOutput.log

A single log file that contains the stdout and stderr from the XippPanel and running Studies is created when xipp is started. The log file,xippOutput.log, is put in the same directory as the xipp executable which by default is at ~/Xipp. This is not ideal since running multiple studies will have all of the output merged into a single file. At this time it is not possible to create separate log files for each running study.

Starting Xipp on MacOS
from a terminal window

xippMac

Ensure that ~/Xipp is on your path or create an alias.
No args to start XippPanel in current directory.
This is actually a Bash shell script that calls the xipp application bundle to start in current directory.
Click 'Studies' to show all Studies in Directory.
Click 'New' to create a new Study, Molecule, Assign Table or Structure.
Click Button next to Path to change current directory.

xipp HprE1_96
xipp HNCACB

Name of NMRPipe NMR Exp such as:
2D 15N HSQC,
3D CBCA(CO)NH stored in separate 2D planes,
3D HNCACB in a single file
On the Mac these form will show the single Exp and starts XippPanel.

Fails on Mac: '**xipp dCBCACONH%03d.DAT**'

The MacOS requires that the file exist before starting xipp. Since dCBCACONH%03d.DAT is not a single file this way of starting xipp is not available under MacOS.

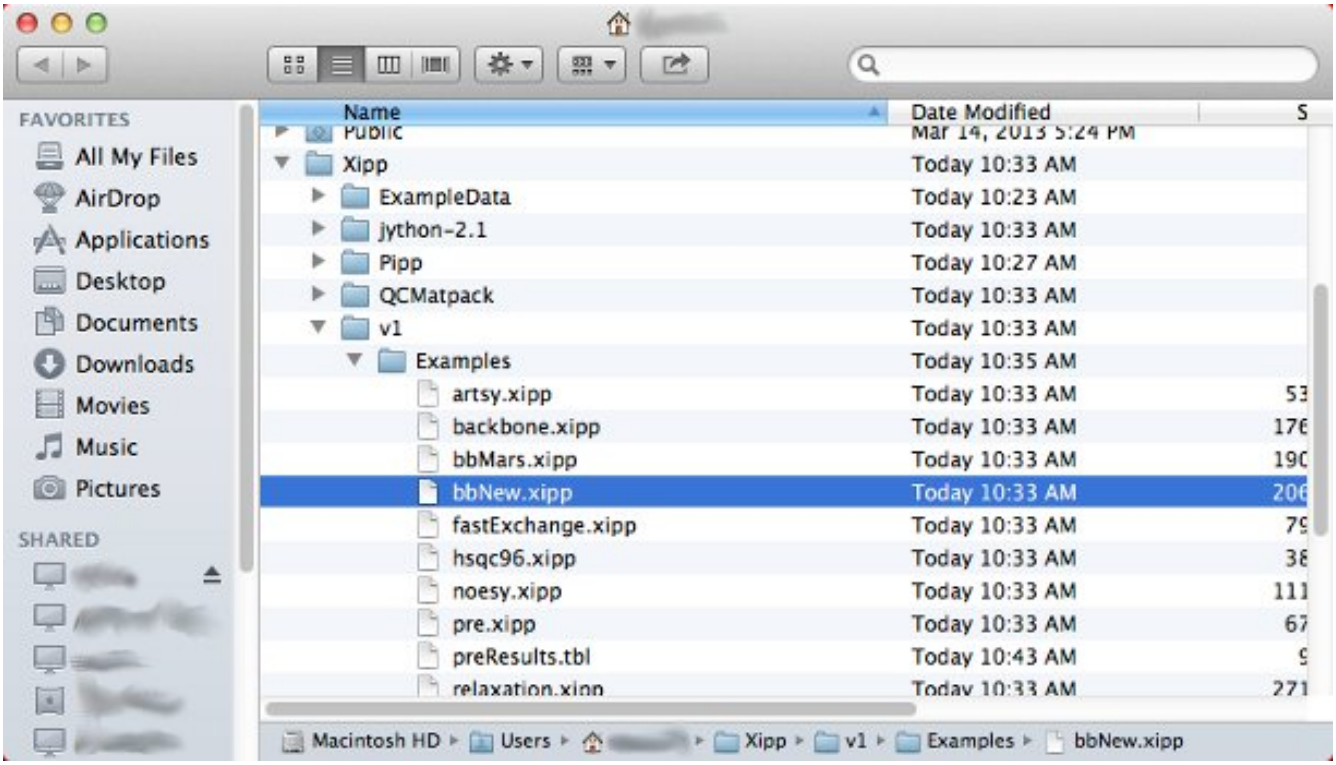
xipp backbone.xipp

Directly start Study backbone.xipp and under MacOS also starts XippPanel

xipp startXipp.py

Start Xipp from Python file by creating and initializing DataServer and GUI Objects.
During development new Java Objects are first implemented by making changes to the startXipp.py and the Python library before implementing in XippPanel.

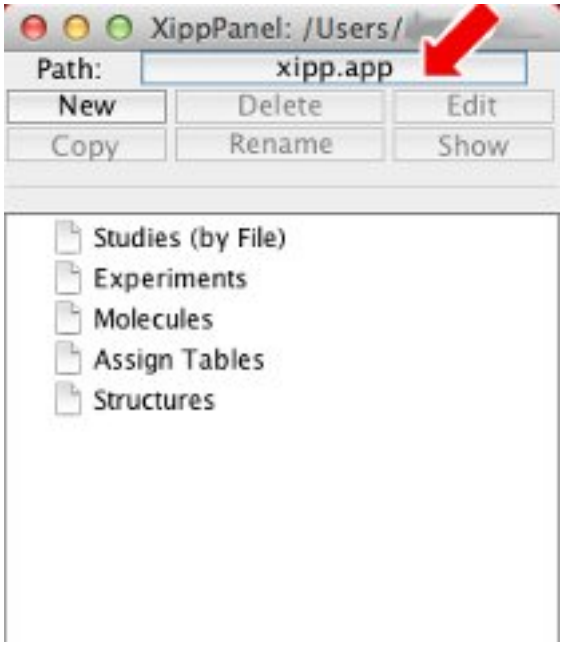
Use Mac Finder



During installation the file extension *.xipp was associated with the xipp application.

Double Click on a *.xipp file in Examples such as bbNew.xipp to show study bbNew and start the XippPanel in the directory with bbNew.xipp.

If xipp is started by doubling clicking the xipp application then only a XippPanel is started in the directory for the bundle which is ~/Xipp/xipp.app by default. You can change directory by clicking the button next to Path.



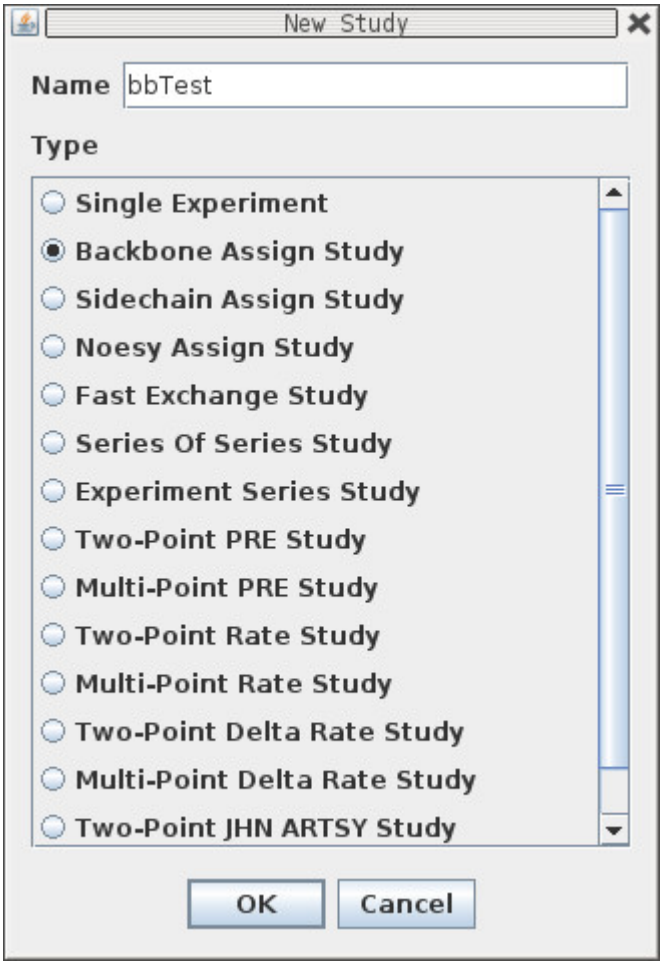
xippOutput.log

A single log file that contains the stdout and stderr from the XippPanel and running Studies is created when xipp is started. The log file,xippOutput.log, is put in the same directory as the xipp executable which by default is at ~/Xipp. This is not ideal since running multiple studies will have all of the output merged into a single file. At this time it is not possible to create separate log files for each running study.

Under MacOS a XippPanel is always started regardless of how xipp starts.

New Study Dialog Panel

This dialog is obtained by clicking the New button on the XippPanel Dialog when either nothing is selected or when a Study is selected.



Currently there are 14 types of Studies:

Single Experiment
Any 2D or 3D experiment.

Backbone Assign Study
Define backbone assignment experiments.

Sidechain Assign Study
Define sidechain assign experiments based.

Noesy Assign Study
Define 3D and 4D NOE experiments.

Fast Exchange Study
Define list of Experiments with Fraction Offset to quickly allow vector peak-picking, ie peak pick residue that changes frequency in a single gesture with all peaks sharing same peak-pick ID and label.

Series of Series Study
Display 1 or more Experiment Series Study.

Experiment Series Study
Define an Experiment Series ^{15}N-HSQC such as T1, T2, T1p or CPMG Disperse. This can also be used to define a Generic Series.

Two-Point and **Multi-Point PRE Study**
Define a Paramagnetic Relaxation Enhancement using two time points or multiple time points.

Two-Point and **Multi-Point Rate Study**
Define a T1, T2 or T1p using two time points or multiple time points.

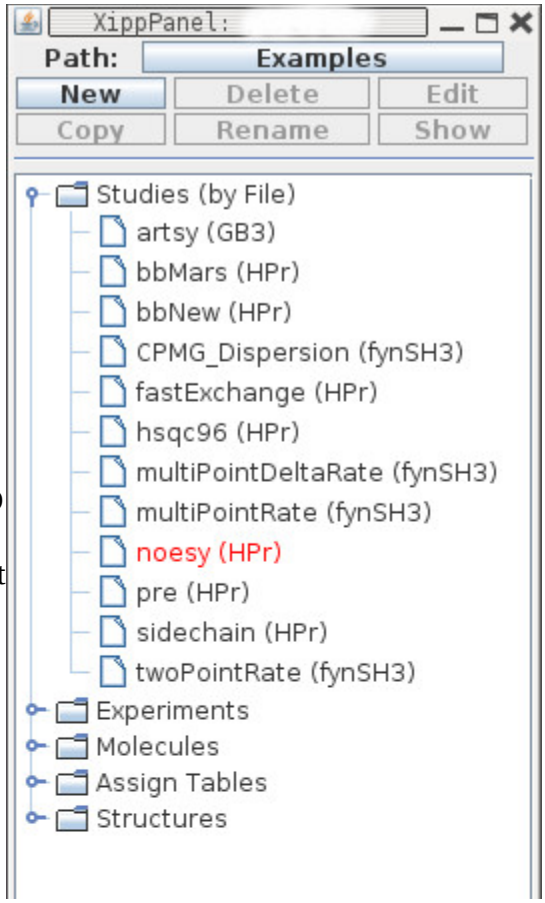
Two-Point and **Multi-Point Delta Rate Study**
Define a delta T2 using two time points or multiple time points.

Two-Point Artsy Study
Defines Reference and Attenuated to calculate ARTSY coupling constant for each residue.

Must enter unique Name and select type of Study to create and show study specific Panel.

The name for a new study will be used to create a file in the current directory that will define the properties of this study. The filename extension .xipp is appended to the name entered in the New Study dialog. The current directory is selected/changed using the Path button on the XippPanel. For Linux the initial current directory is the directory in which the xipp command was executed.

Editing Study Properties



The 'Studies (by File)' node lists all of the study files that exist in Path which are defined by the *.xipp files.

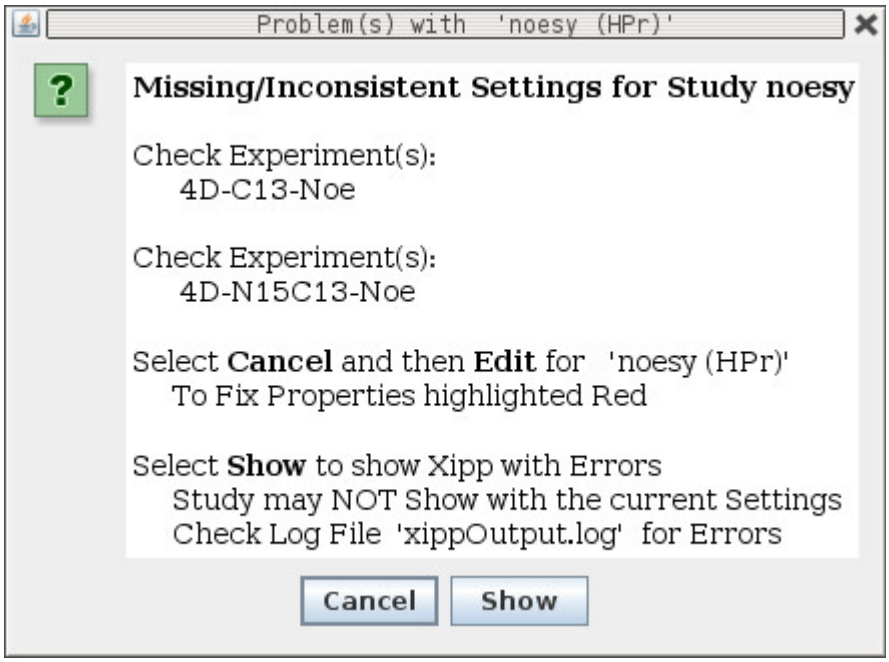
The list is sorted by study name with a user settable group name shown in parenthesis. The group name defaults to the username creating the study, but the name can be easily changed.

Each study name must be unique within a directory since the study name is also the base name of the file with .xipp as the extension.

The noesy (HPr) study is shown in red to indicate that there is a problem with the properties that may prevent the Study from being shown. The noesy study defines the 3D 13C-Noesy, 15N-Noesy, the 4D 13C,13C-Noesy and the 4D 15N,13C-Noesy. The problem arises from the 4D Noesy experiments not being downloaded so they are not present in the ExampleData directory.

The Warning message below is displayed when the noesy study is selected and Shown by clicking the Show button. A similar Warning message will be displayed whenever a study is attempted to be shown that has problems.

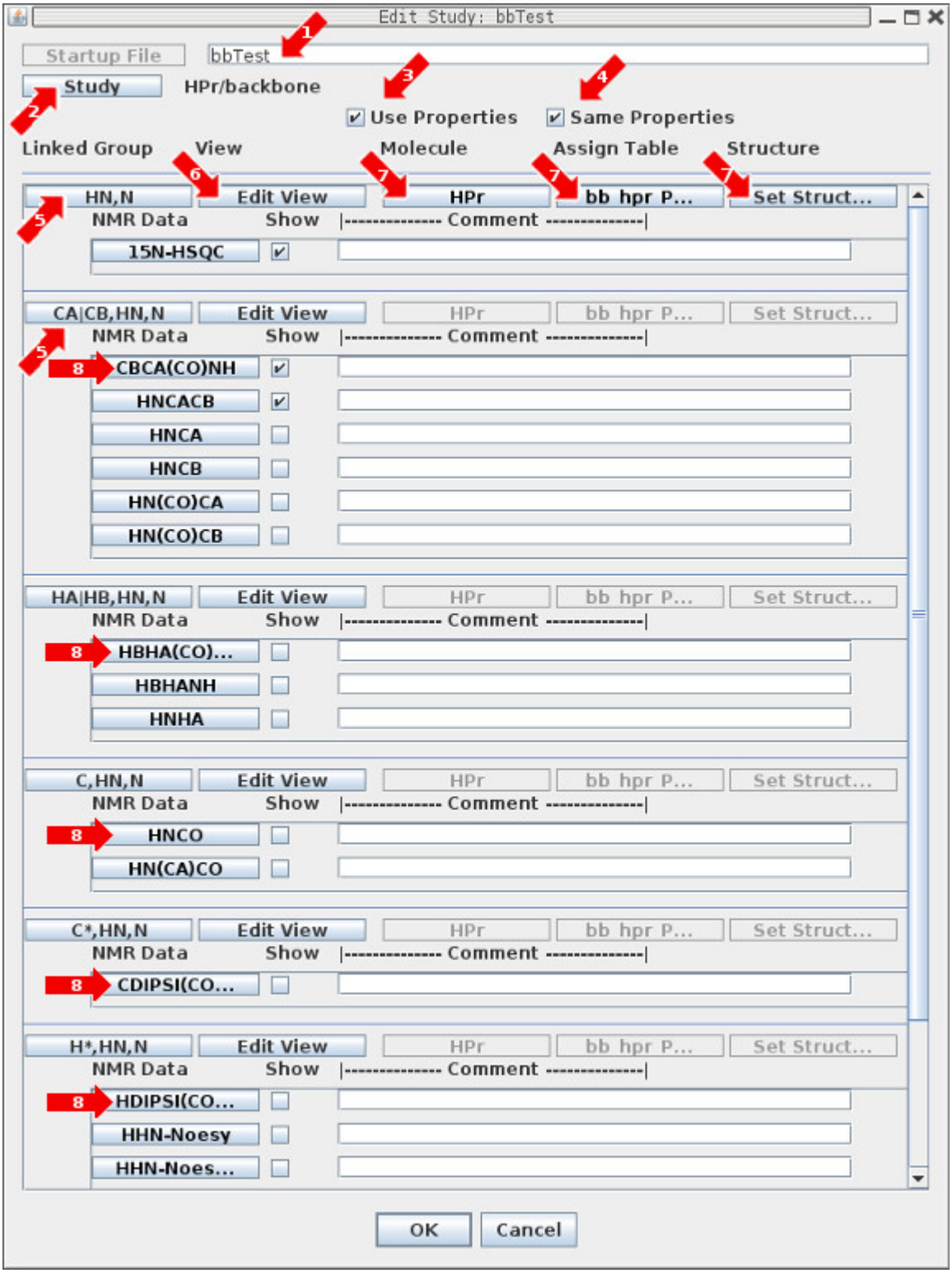
Note that the warning says that the 'Study **may** NOT show'. It does not say that the study will not show. The noesy study will show with only the 3D noesy experiments. At least one NMR experiment must be defined to show a study. Experiments that are not defined are ignored.



Backbone Assign Study Dialog

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with Backbone Assign Study selected.
2. By clicking on the Edit button on the XippPanel when a Backbone study is selected.



Backbone Assign Study

Each type of study has its own Dialog Panel. The study dialog panels for Backbone Assign, Sidechain Assign and Noesy Assign all share the same format in which the NMR experiments are grouped by ability to be overlayed. The name of the Linked Group identifies the atoms that are overlayed.

1: The name of the study is shown at the top and can be changed which will create a new *.xipp file. Changing the study here is equivalent to copying the *.xipp file. Unfortunately the XippPanel does not update the list of Studies when the file copied using a terminal. Clicking the old study name brings up the new study and you must close the XippPanel and restart xipp to show the old and new study.

2: Click the Study button to change the two user settable names for the study.

3: 'Use Properties' button controls whether the study will use Molecules, Assign Tables or Structure. When toggled off none of these properties are used so that when peaks are created the user sets a label for each peak instead of selecting an assignment from a list suggested by Xipp.

4: The 'Same Properties' check box controls whether the Linked Groups all share the same properties or not.

5: Currently the Linked Group buttons such as HN,N and CA|CB,HN,N do not do anything.

6: The 'Edit View' button for a linked group becomes active after the first NMR experiment is defined and brings up the Linked Group View Properties described below.

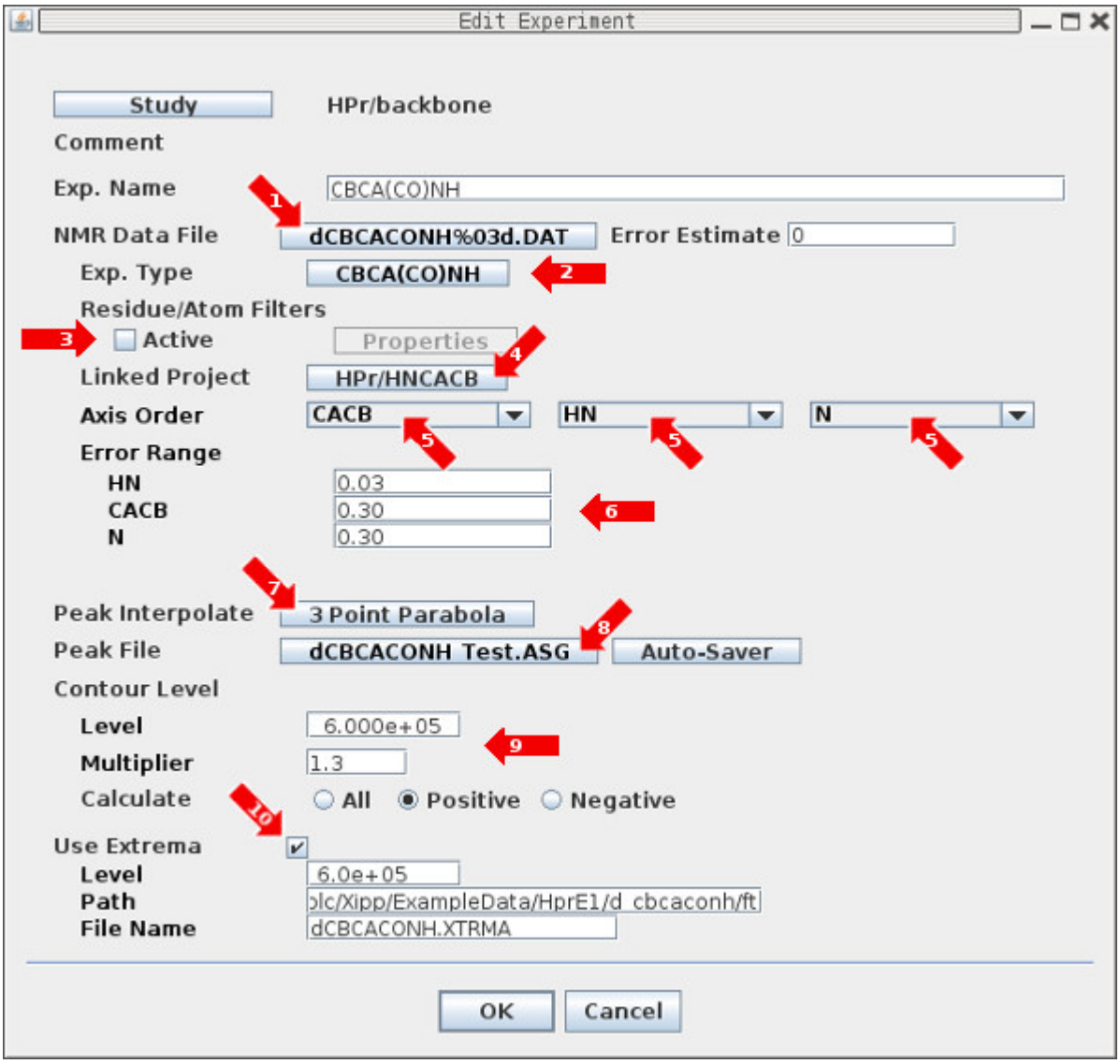
7: The Molecule, Assign Table and Structure buttons for each linked group bring up the Select/Create Dialog for Molecule, Assign Table and Structure respectively.

8: Clicking the NMR Data buttons under a linked group brings up the Edit Experiment Dialog used to define the location and properties specific to a single NMR experiment. Only click on experiments for which you have data. Currently there is no way to add new experiments to a linked group. There are defined relationships between some experiments that will cause problems if the data for an HNCA were put into the CBCA(CO)NH NMR Data button.

Clicking OK at the bottom of the Edit Study Dialog will save all of the properties into the file based on the study name, ie bbTest.xipp in this example.

Note the text on a button will be red when the properties that are accessed by that button are not correctly set. Clicking OK with incorrectly set properties will bring up a Warning Dialog asking if you want to Fix the problem(s) (i.e. re-show the dialog) or Ignore the problem(s) and save the properties with the problems. Incorrect properties may not show correctly and another pop-up window will warn when a Study with incorrect settings is attempted to be shown. Some problems such as undefined Experiment with the Show check box clicked on will actually Show OK, but the warning message is still displayed.

NMR Data Experiment Dialog



The NMR Experiment Dialog is used to identify the NMR data such as (1) File(s), (2) Exp. Type,, (5) Axis Order, (6) Error Range, (8) Peak Pick File, (9) Contour Level, and (10) Extrema Level and File if used. **The (1) NMR Data File must always be set.** The default value for all of the other properties is usually OK except when (10) Extrema are needed for locating 3D Symmetry or locating Sequential Spins in Backbone assignment experiments.

NMR Data Experiment Dialog

1: Click the NMR Data File button to bring up the NMR Data File Chooser to select the file or file-set. Initially the text on this button will be red indicating that the file has not been set. There are no defaults for this.

2: The Exp. Type identifies the type of NMR experiment and should rarely be changed. This defines the Atoms that are observed and the relationships between the atoms. For the CBCA(CO)NH experiment the observed atoms are Cα,Cb on one axis, HN on a second axis and N on the third axis. The HN and N must be bonded and the residue of Cα or Cβ must be (i-1) relative to N.

3: Residue/Atom Filters should only be used with samples that have mixed isotopic labeling. For example a sample with HPr(^{15}N,^{13}C) and EIN(^{14}N,^{12}C) . You can identify by residue which atoms can be observed (ie HPr) and which can not be observed (ie EIN) for each axis. A molecule in Xipp is defined as a single peptide using spacer residues (ie G's) between EIN (residues 1-259) and HPr (residues 301-385).

4: The Linked Project identifies a project that is linked to this project and should rarely be changed. This is used by Xipp when doing assignments. This is automatically set based on the Study and should automatically update when project names are changed.

5: The Axis Order defines what atoms are observed along each axis. For triple resonance experiments all axis are automatically set based on the Exp. Type and the spectrometer frequency from the NMR Data File. For double resonance experiments one or more axis will have to be manually set. The button Data Reference on the NMR Data File Chooser displays the NMRPipe header information.

6: The Error Range defines a maximum cut-off in making assignments. The defaults are OK for most backbone and sidechain assignment experiments.

7: The Peak Interpolate button brings up the Peak Pick Options Dialog that allows setting the Interpolation and the size in data points of the matrix that is read in for every peak-pick.

8: Clicking the Peak File button brings up the Peak Pick File Chooser Dialog. The initial default value for the peak-pick file name is the base name from the NMR Data file with the extension replaced with .ASG and .PCK.

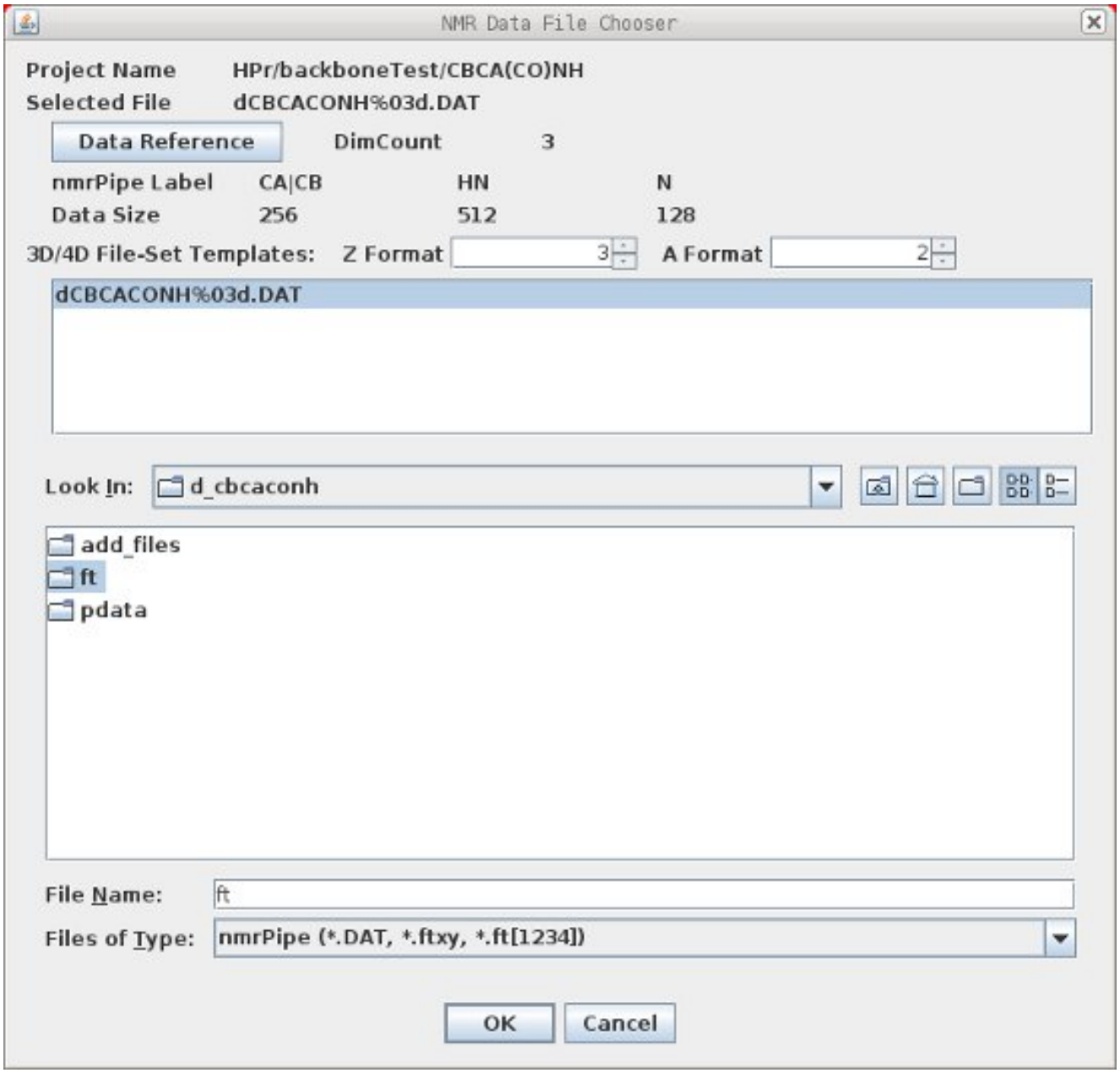
9: The Contour Level options set the threshold and multiplier for contouring the data. These values can be changed while Xipp is running, but new settings in Xipp are not saved in the the *.xipp file so are not remembered when Xipp is restarted. You must make the changes in this dialog to be permanent.

10: By default Use Extrema is off. This should be enabled when 3D Symmetry or locating Sequential Spins in Backbone assignment experiments is needed. When Use Extrema is clicked on the Level is automatically set to the current value of the Contour Level.

Note the text on a button will be red when the properties that are accessed by that button are not correctly set. Initially the NMR Data File text will be red to indicate that the NMR Data needs to be set.

NMR Data File Chooser

This dialog is obtained by clicking the NMR Data File button from the NMR Data Experiment Dialog.



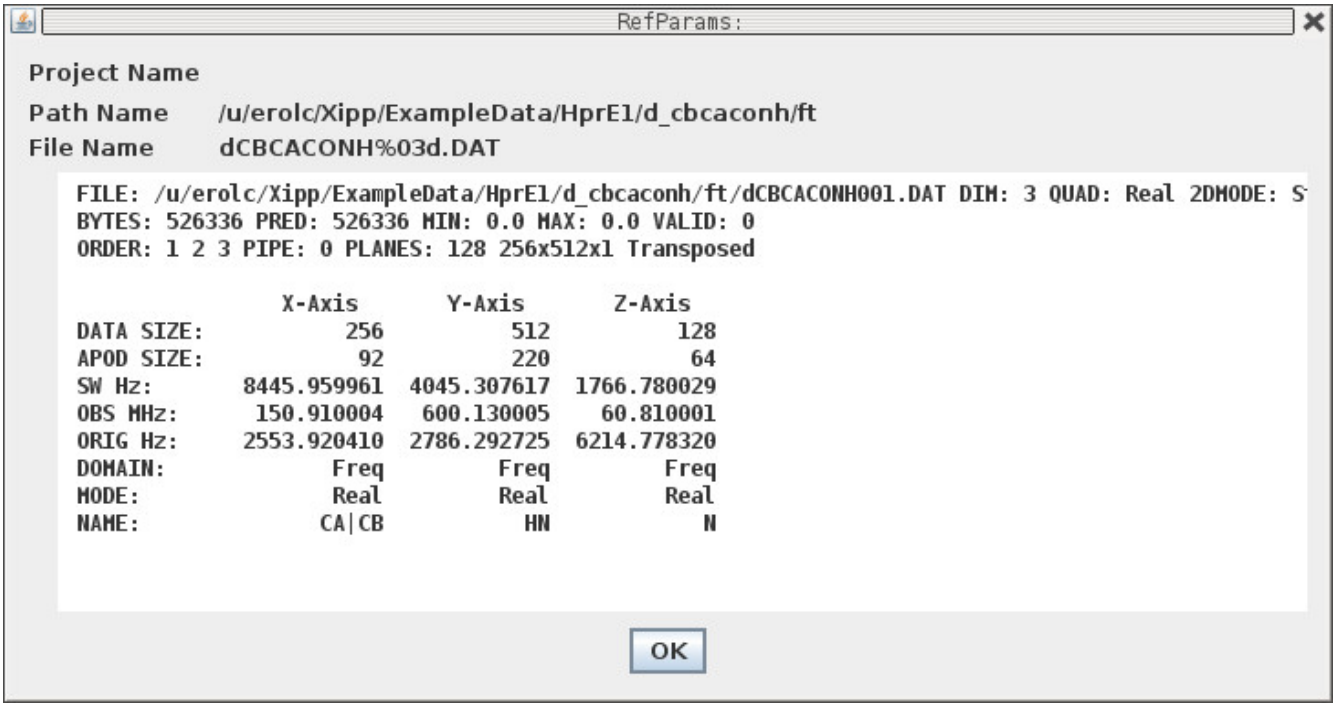
When the NMRPipe file or file set is selected the DimCount, nmrPipe Label and Data Size are updated from NMRPipe header.

Clicking the button Data Reference brings up the RefParams Dialog using the NMRPipe header from the first plane of the selected file-set in a separate non-modal window. Since the NMR Data File is a modal window the RefParams Dialog is shown under the NMR File Chooser. You can not close the RefParams Dialog until the NMR File Chooser is closed.

RefParams Dialog

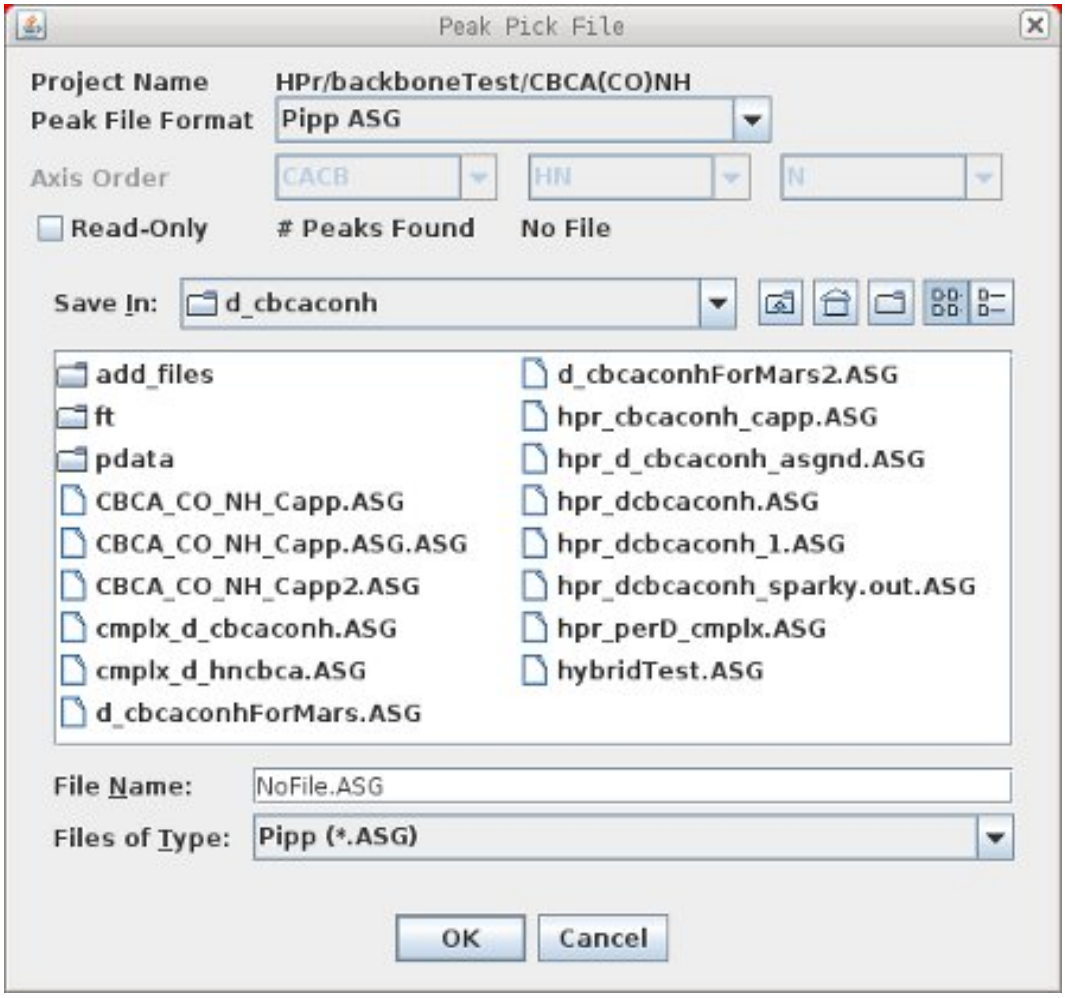
This dialog is obtained by clicking on the Data Reference button from the NMR Data File Chooser.

Since this is a non-Modal dialog and the NMR Data File Chooser is a modal dialog the RefParams Dialog is shown under the NMR Data File Chooser and the NMR Data File Chooser must be closed first.



Peak Pick File Chooser

This dialog is obtained by clicking on the Peak File button from the NMR Data Experiment Dialog.

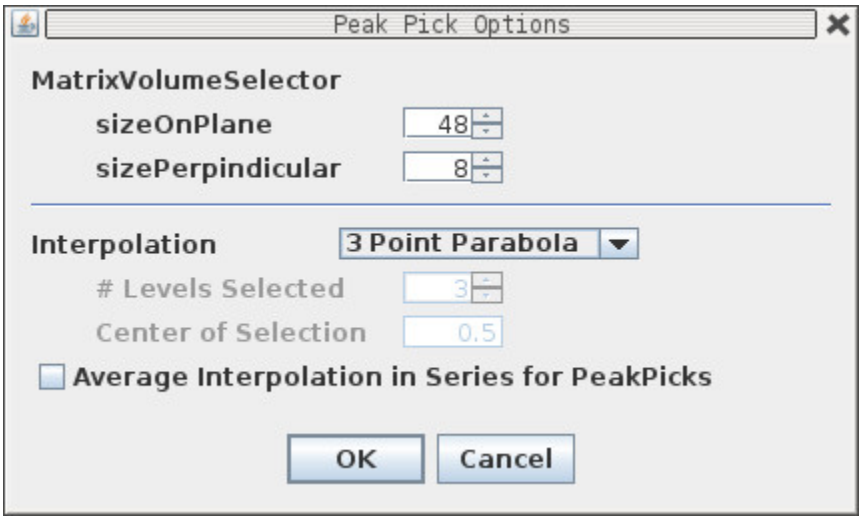


The # Peaks Found is updated whenever a valid Peak-Pick file is selected.

The Pipp ASG format is well tested whereas the Sparky Peaks is not well tested.

I strongly suggest using mainly the Pipp ASG format.

Peak Pick Options Dialog



The default options are usually good for most NMR Experiments.

The MatrixVolumeSelector sizeOnPlane and sizePerpindicular defines a sub-matrix volume that is read in and centered on the mouse position when doing peak picking. If the user did not hold the Crtl key down while peak-picking then Xipp finds a nearby local extrema by walking up the steepest gradient within the sub-matrix volume. For highly zero-filled data it might be necessary to increase sizeOnPlane to ensure that the local extrema is within the sub-matrix volume.

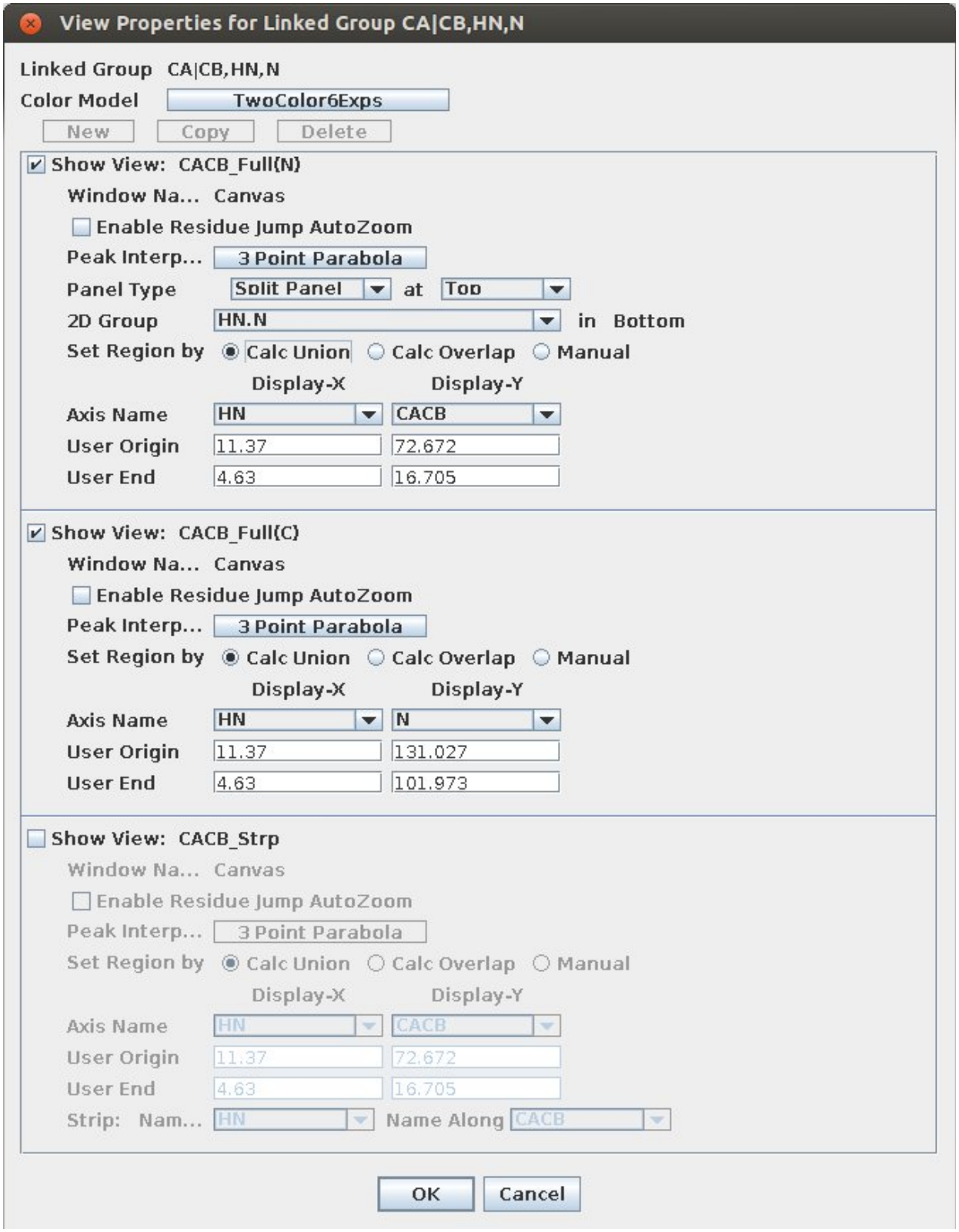
There are three type of interpolation:

- 3 Point Parabola
  - Start at mouse position and go up the steepest gradient to find local extrema. Fit the top 3 points to a parabola and report top of the parabola as the peak position for each axis.
- Contour Average
  - Start at mouse position and go up the steepest gradient to find local extrema. Average the X,Y position of contours that encircle the local extrema at Center of Selection fraction of peak height to define peak position on contoured X, Y plane. This usually works best with well resolved peaks and high zero-filling which requires sizeOnPlane to be increased.
- Same Position
  - Use the same X, Y PPM position as determined from earlier Exp. This can only be set for Studies where multiple experiments are overlayed and the first experiment can not use Same Position.

When the Average Interpolation in Series for PeakPicks is checked Xipp will average the X, Y value obtained from all experiments and use that point in the experiments to get the intensity from each experiment. If 3 Point Parabola is the Interpolation and Average Interpolation is enabled then the position of all the peaks will be the average of the 3 Point Parabola from all the experiments that are overlayed. This should never be used with Backbone, Sidechain or Noesy Studies since it hides differences in chemical shift that might help identify mis-assignments. This is designed for Experiment Series to select the same point in all 2D ^{15}N-HSQC experiments based on the average position from all experiments.

Linked Group CA|CB,HN,N Edit View Dialog

This dialog is obtained by clicking on the Edit View button from the Edit Study: Backbone Assign Dialog.



Linked Group CA|CB,HN,N Edit View Dialog

The Edit View Panel for the linked group CA|CB,HN,N has 3 possible views:

CACB_Full(N)

This has CA,CB and HN on the displayed 2D plane with ^{15}N defining the plane.
Click the Check Box Enable Residue Jump AutoZoom to have xipp automatically zoom to assigned peaks after a residue jump.
Do NOT use Peak Interpolate here. I moved it to the NMR Experiment panel so that different experiments in a series can have different interpolations.
Panel Type can be set to 'One Pane' or 'Split Panel'. When set to 'Split Panel' a 2D such as an ^{15}N-HSQC can be shown in a lower panel whose ^{15}N is kept in sync with ^{15}N of 3D experiments shown in upper panel. Select 'One Panel' to just show the 3D experiments in a single panel.
2D Group defines the Linked Group to show in the lower panel.
Axis Name should be set with HN and N. The full display region can be set to Union, Overlap or manually set by 'Set Region by' buttons and if Manual selected entering desired region. Usually the best choice is Union since that calculates the Region as a union from all NMR experiments. The units for User Origin and End are PPM.

CACB_Full(C)

This has N and HN on the displayed 2D plane with ^{13}C of CA/CB defining the plane.
Click the Check Box Enable Residue Jump AutoZoom to have xipp automatically zoom to assigned peaks after a residue jump.
Do NOT use Peak Interpolate here. I moved it to the NMR Experiment panel so that different experiments in a series can have different interpolations.
Axis Name should be set with HN and N. The full display region can be set to Union, Overlap or manually set by 'Set Region by' buttons and if Manual selected entering desired region. Usually the best choice is Union since that calculates the Region as a union from all NMR experiments. The units for User Origin and End are PPM.

CACB_Strp

Strips should not be used at this time. I plan on replacing the currently broke Strip feature with a better tool to handle backbone assignments with triple resonance data and ^{15}N NOESY experiments.

Molecule Select/Create Dialog

This dialog is obtained by clicking on the Molecule button from the Backbone Assign Dialog. Note you must first enable properties by clicking 'Use Properties' check box on.

The Select/Create Molecule Dialog shows all of the molecules that have been created for all studies defined by *.xipp files in this directory.

The list is sorted by molecule name with the study name shown in parenthesis.

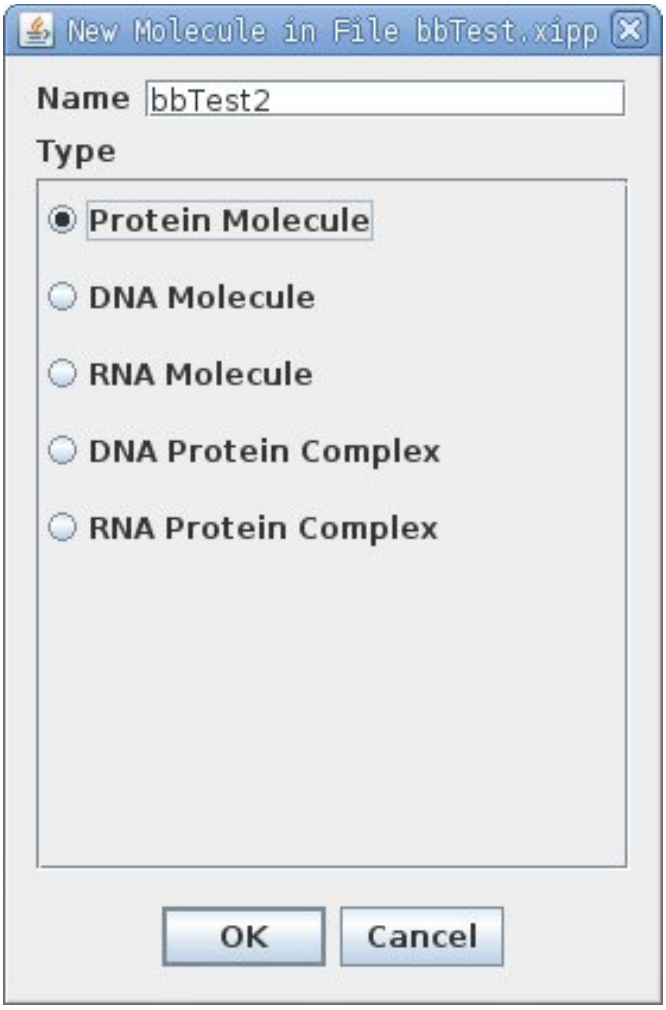
Each molecule name must be unique within its own study, but the same molecule name can be used in different studies.

Currently there are 5 types of Molecules:

- Protein Molecule
  - Defined by sequence using single letter codes.
- DNA Molecule
  - Defined by DNA sequence using single letter codes.
- RNA Molecule
  - Defined by RNA sequence using single letter codes.
- DNA Protein Complex
  - Protein sequence uses upper case characters for single letter codes and DNA uses lower case characters for single letter codes.
- RNA Protein Complex
  - Protein sequence uses upper case characters for single letter codes and RNA uses lower case characters for single letter codes.

New Molecule Dialog

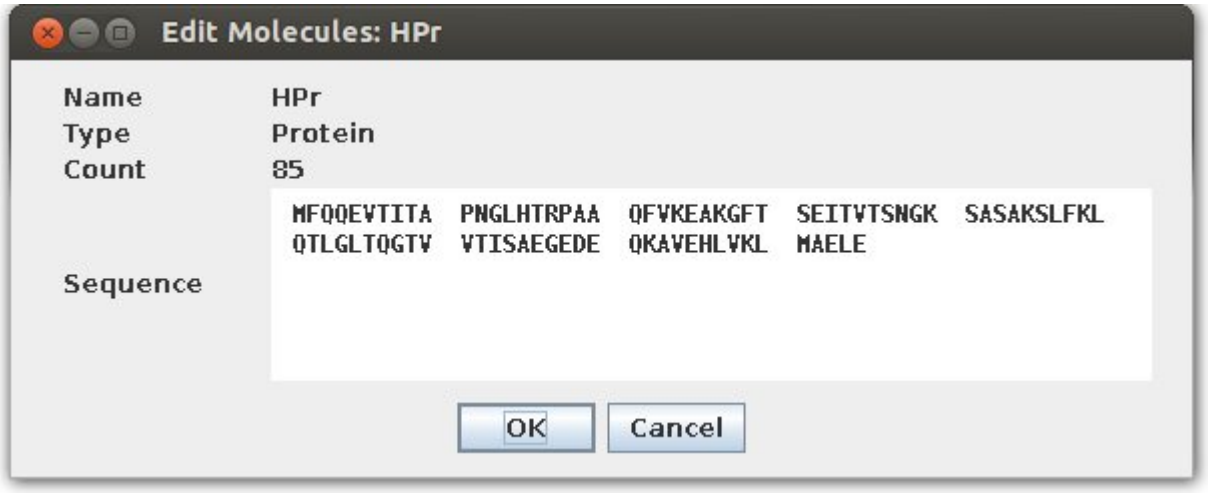
This dialog is obtained by clicking on the New button from the Select/Create Molecule Dialog.
The Name for the molecule must be unique within this study but can be the same name of a molecule used in another study.



Molecules Dialog: Protein

This dialog can be obtained in two ways:

1. By clicking on the New button from the Select/Create Molecule Dialog.
2. By clicking on the Edit button from the Select/Create Molecule Dialog.



You can either type in your sequence or use your mouse to cut and paste your sequence from a file or web page. This dialog only accepts single letter amino acid codes.

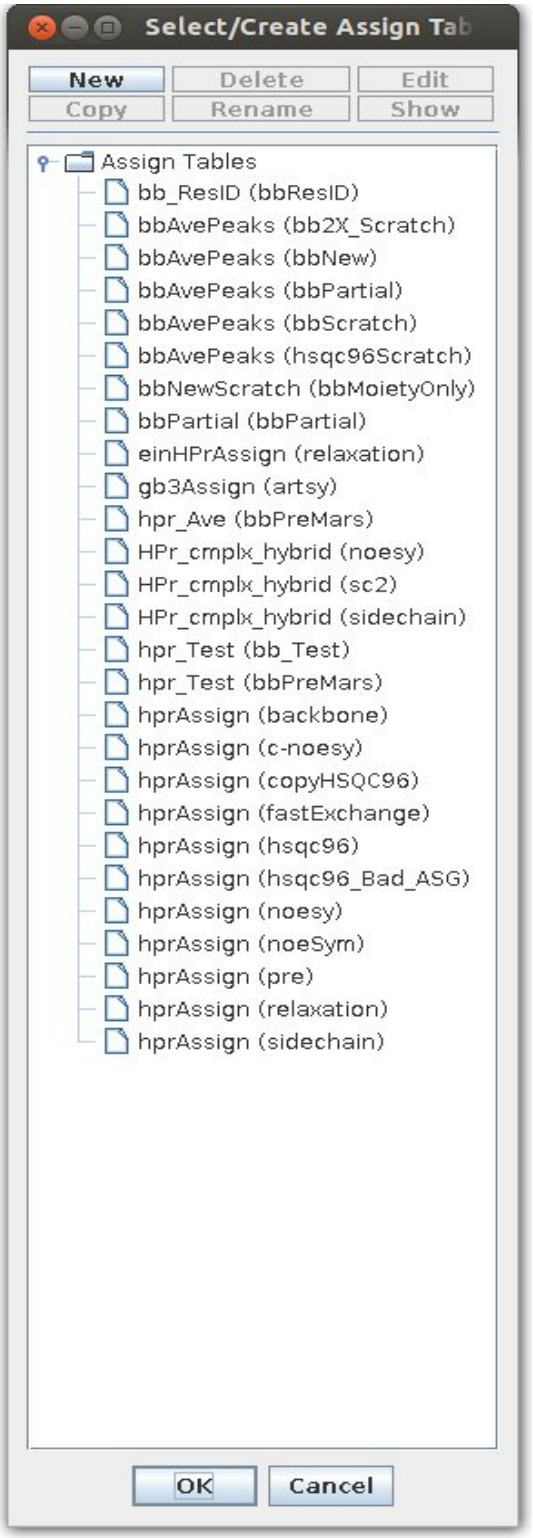
To create multi-chain sequences enter the longest sequence first then pad with G or A up to nearest multiple of 100. For the complex EIN (1 → 259) with HPr (301-> 385) I used:

MISGILASPG IAFGKALLLK EDEIVIDRKK ISADQVDQEV ERFLSGRAKA SAQLETIKTK AGETFGEEKE AIFEGHIMLL EDEELEQEII ALIKDKHMTA DAAAHEVIEG QASALEELDD EYLKERAADV RDIGKRLLRN ILGLKIIDLS AIQDEVILVA ADLTPSETAQ LNLKKVLGFI TDAGGRTSHT SIMARSLELP AIVGTGSVTS QVKNDDYLIL DAVNNQVYVN PTNEVIDKMR AVQEQVASEK AELAKLKDRA AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA AAAAAAAAAA
MFQQEVTITA PNGLHTRPAA QFVKEAKGFT SEITVTSNGK SASAKSLFKL QTLGLTQGTV VTISAEGEDE QKAVEHLVKL MAELE

This same trick can be used with Protein DNA complexes. Just remember to use lower case for the DNA and RNA single letter code.

Assign Table Select/Create Dialog

This dialog is obtained by clicking on the Assign Table buttons from the Backbone Assign Dialog. Note you must first enable properties by clicking 'Use Properties' on the Backbone Assign Dialog..



The Assign Table Select/Create Dialog shows all of the assignment tables that have been created for all studies defined by *.xipp files in this directory.

The list is sorted by Assign Table name with the study name shown in parenthesis.

Each Assign Table name must be unique within its own study, but the same Assign Table name can be used in different studies.

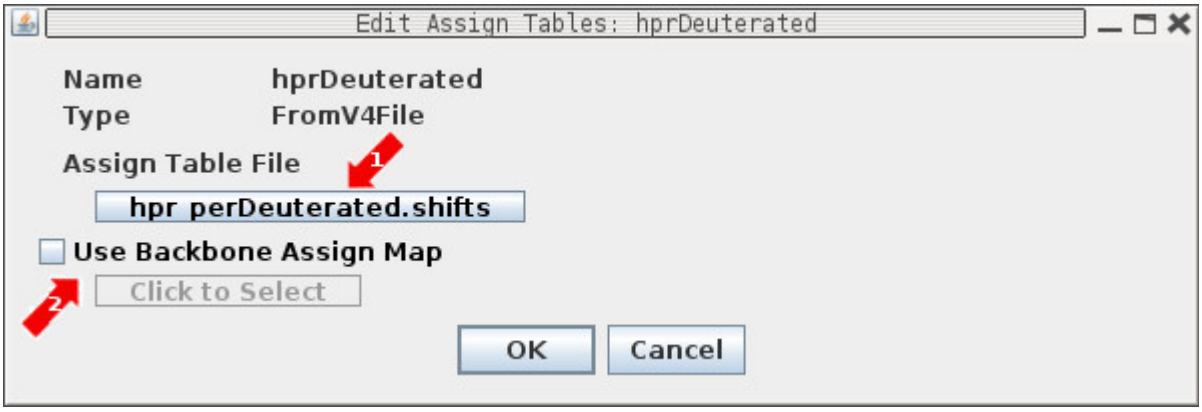
Currently there are 3 types of Assign Tables:

- Assignment File (PIPP V4)
  - Single file in PIPP format defining assignment table, ie a *.shifts file.
- Average Assigned Peaks into …
  - Assigns are dynamically averaged from all assigned peaks in chosen Experiments.
- Hybrid Assignment Table
  - **Do NOT use. This is not well tested.**
  - Merges list of assign tables to form 1 table.
  - Assigns from first table take precedence over assigns from tables lower in list.

Assign Table Dialog: FromV4File

This dialog can be obtained in two ways:

1. By clicking on the New button from the Select/Create Assign Table Dialog.
2. By clicking on the Edit button from the Select/Create Assign Table Dialog.



The FromV4File defines an Assignment Table from a file in the format as used by PIPP Version 4.

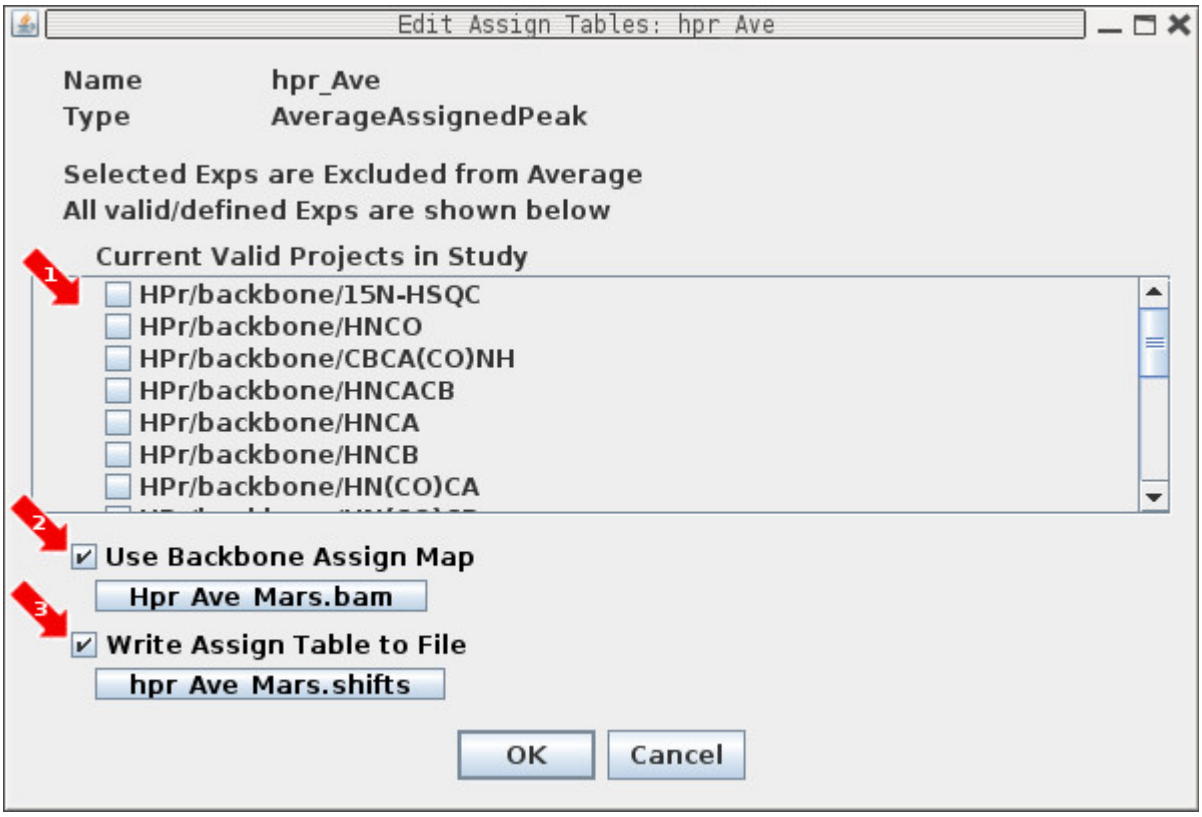
(1) Click Button to bring up Assign Table File Chooser.

(2) Enable Backbone Assign Map only for creating assignments from scratch with Backbone Assign Study. The Backbone Assign Map creates a file that maps between unassigned Spin-Systems and Residues.

Assign Table Dialog: AverageAssignedPeak

This dialog can be obtained in two ways:

1. By clicking on the New button from the Select/Create Assign Table Dialog.
2. By clicking on the Edit button from the Select/Create Assign Table Dialog.



The AverageAssigned Peak defines a dynamic Assignment Table that is the average of all assigned Peak-Picks. As each Peak-Pick is assigned the Assignment for the atoms being assigned are updated with a new average. By default all Projects (ie NMR experiments) are used in the average.

(1) This is a list of all possible Projects. Selecting a Project will remove that NMR experiment from participating in defining the average assignment. By default nothing is selected so that assigned peaks from all defined Projects will be averaged to create the AverageAssignedPeak Assignment Table. **Only select a Project to remove it from the average.**

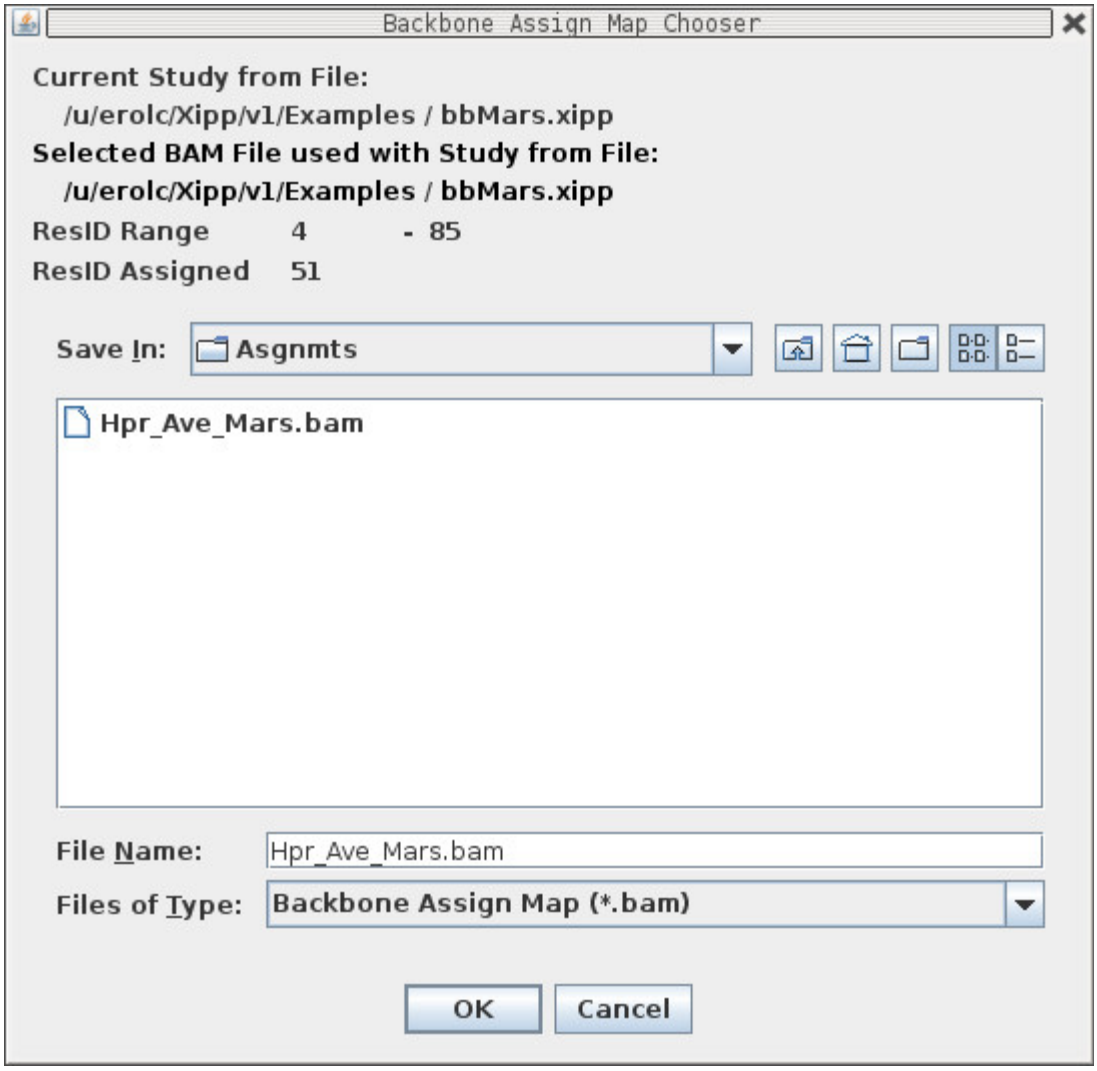
(2) The Use Backbone Assign Map check box when checked indicates that a Backbone Assign Map is being used to create backbone assignments from scratch for Backbone Assign Study only. For all other studies this should not be used. Clicking the Button brings up the Backbone Assign Map File Chooser.

(3) The Write Assign Table check box when selected will write out a PIPP V4 format shifts file that can be read in later for other studies such as Sidechain or Noesy Assign study. The AverageAssignedPeak never reads in this file. Clicking the button brings up the Assign Table File Chooser.

Backbone Assign Map File Chooser

This dialog can be obtained in two ways:

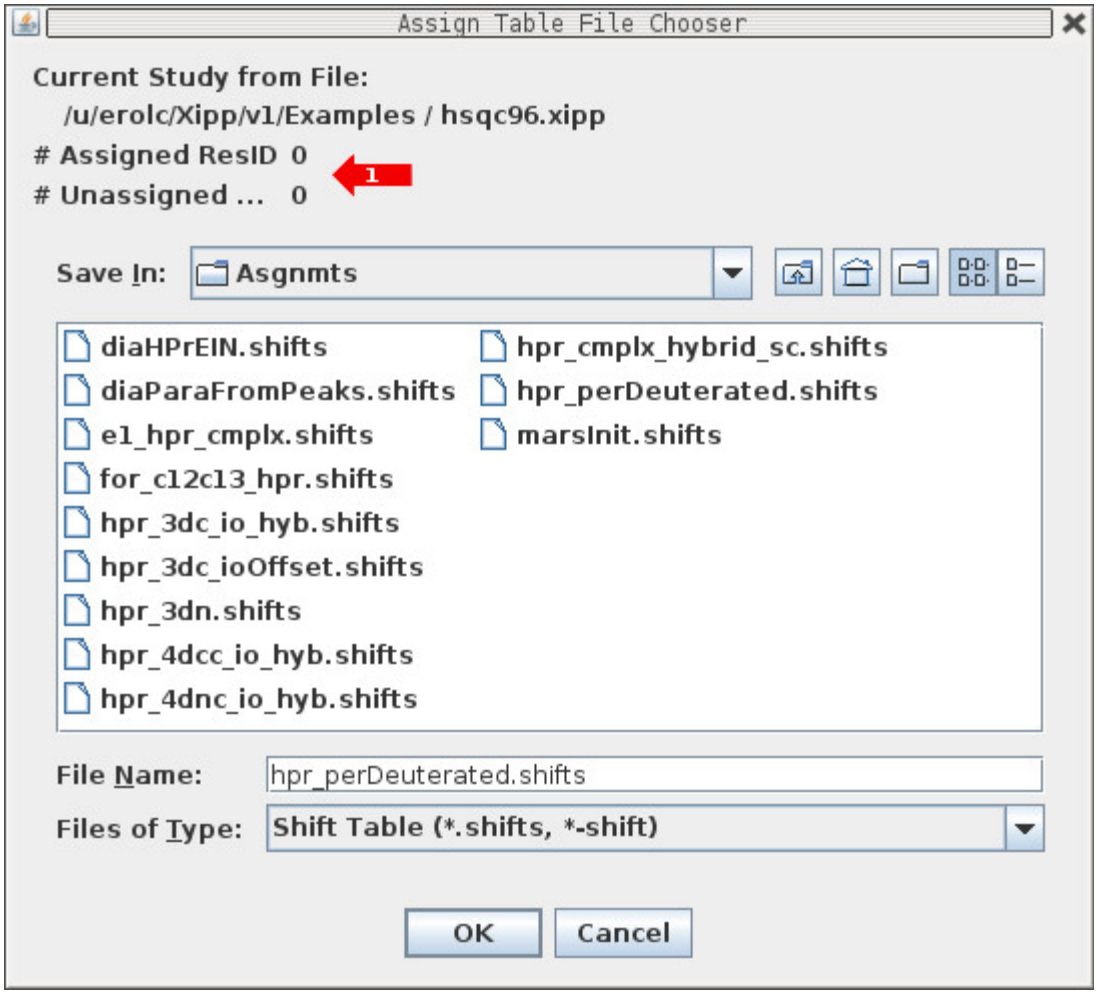
1. By clicking on the Backbone Assign Map button from the Assign Table Dialog: FromV4File
2. By clicking on the Backbone Assign Map button from the Assign Table Dialog: AverageAssignedPeak.



Assign Table File Chooser

This dialog can be obtained in two ways:

1. By clicking on the Assign Table File Button from the Assign Table Dialog: FromV4File
2. By clicking on the Write Assign Table to File from the Assign Table Dialog: AverageAssignedPeak.

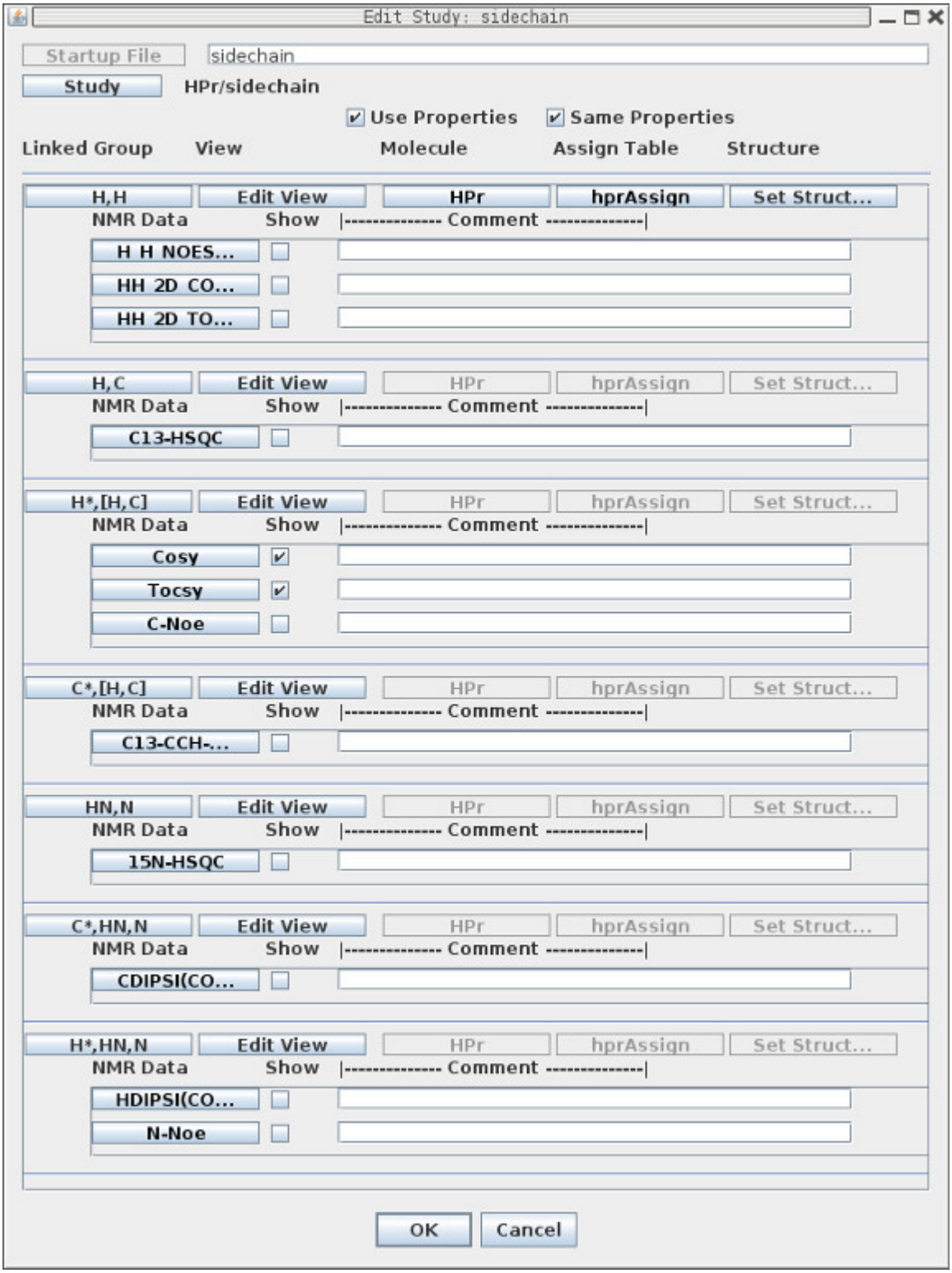


(1) The Assigned ResID and Unassigned always show 0. I need to add a counter so these are updated.

Sidechain Assign Dialog

This dialog can be obtained in two ways:

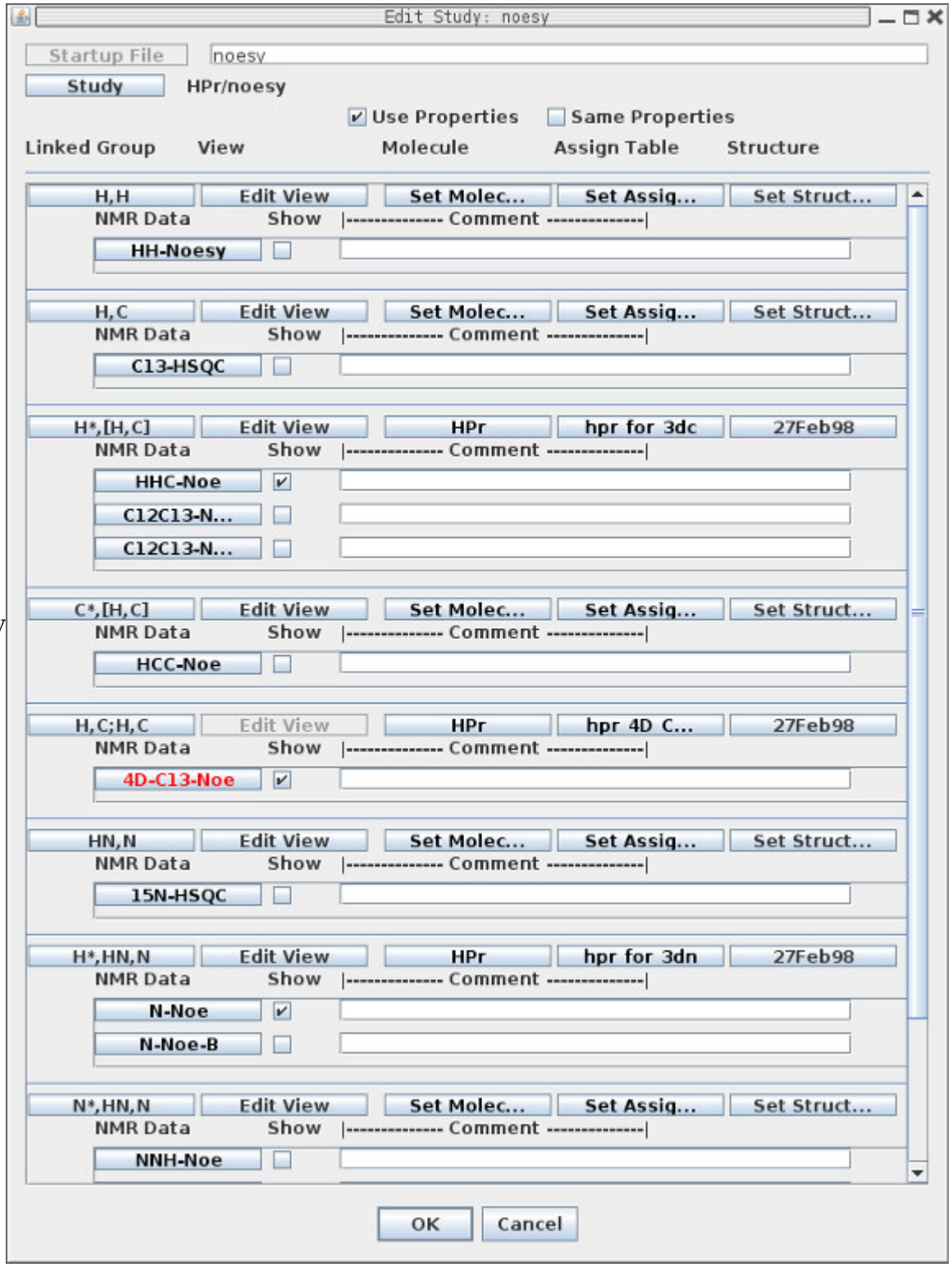
1. Creating new study from New Study Dialog Panel with Sidechain Assign Study selected.
2. By clicking on the Edit button on the XippPanel when a sidechain study is selected.



Noesy Assign Study Dialog

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with Noesy Assign Study selected.
2. By clicking on the Edit button on the XippPanel when a Noesy study is selected.



The 4D Experiments are shown in Red only if the data has not been downloaded.

Uncheck the Show next to 4D Experiments to stop the Warning messages.

Note there is a 4D-15N,13C that must also be unchecked.

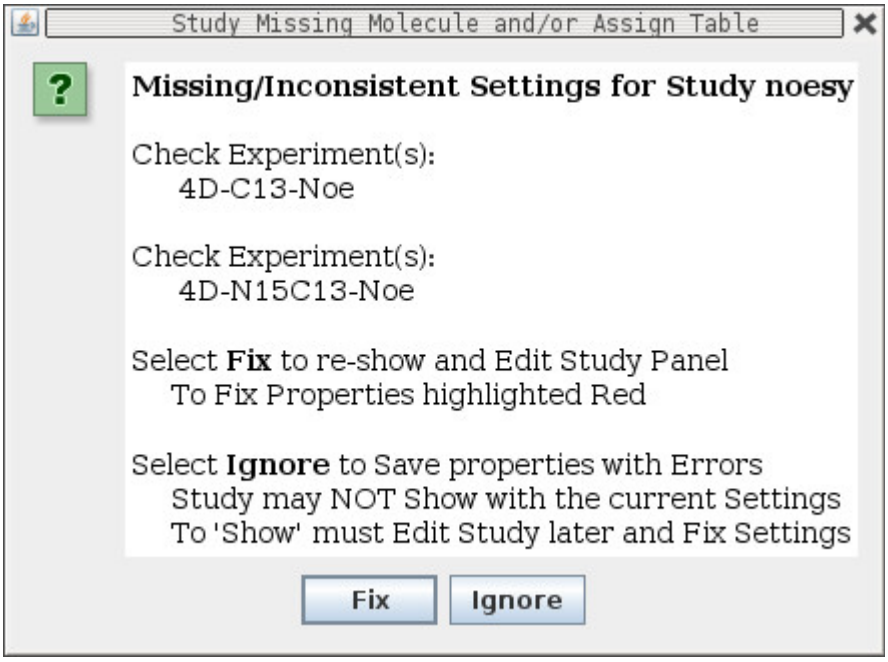
Sidechain Assign Dialog
Noesy Assign Dialog

The layout and response of the buttons for a Sidechain Assign Dialog and the Noesy Assign Dialog is identical to the Backbone Assign Dialog. The main difference is the names of the NMR experiments and linked groups.

Refer to the page 'Backbone Assign Study Dialog' for a description of the buttons.

Clicking OK at the bottom of the Edit Study Dialog will save all of the properties into the file based on the study name such as bbTest.xipp, sidechain.xipp and noesy.xipp in these examples. If there are any problems with the settings then a Warning Message will pop up after clicking OK.

Warning Message from Noesy Assign Dialog due to Missing 4D Experiments

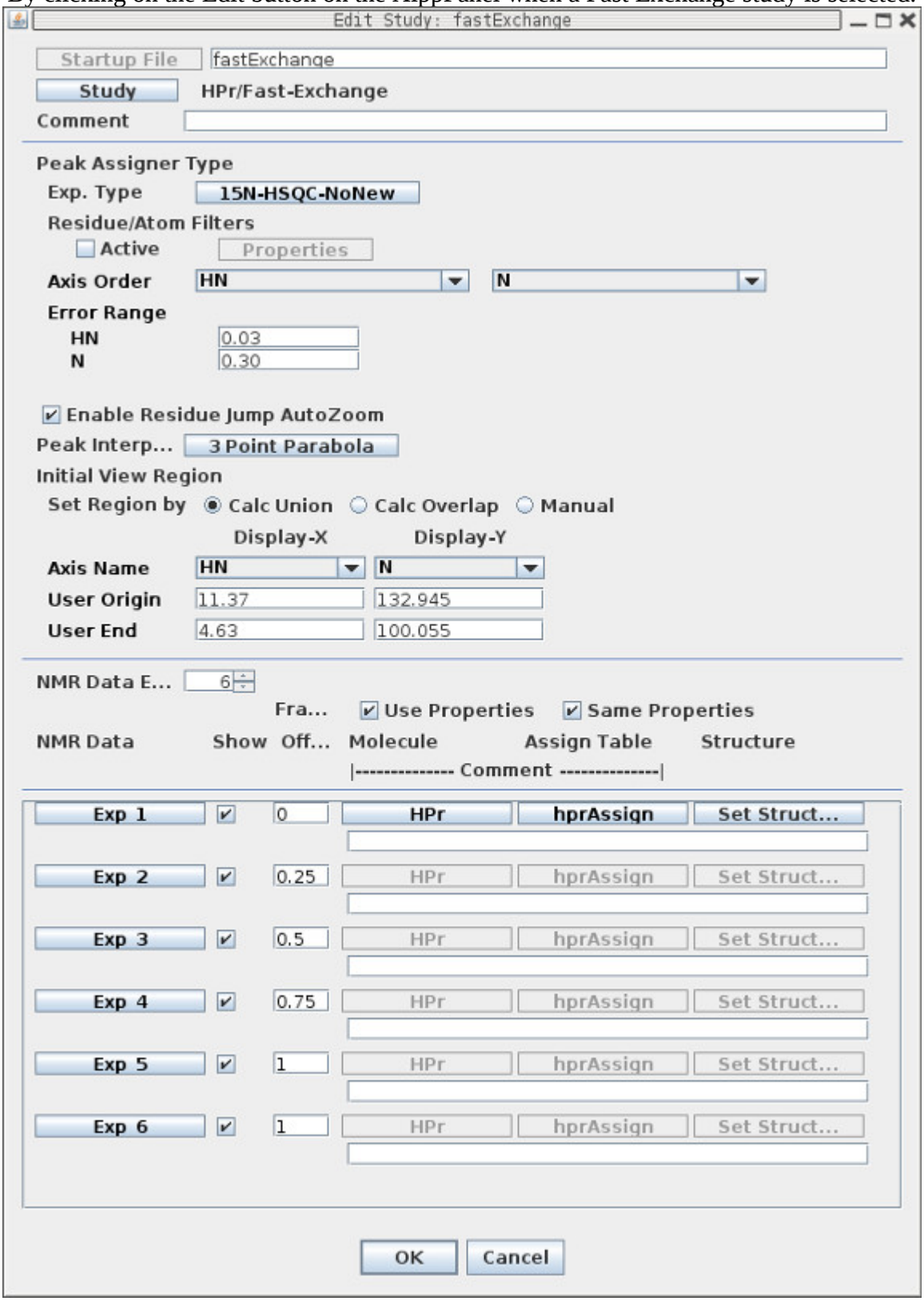


The Warning message is self explanatory. Note there is a similar message that appears when trying to Show a Study with problems except that Fix get replaced with Cancel and Ignore is replaced with Show. This specific Warning can be ignored and the Study will Show because Xipp will ignore missing Experiments when showing a Study. To get rid of the annoying warning messages simply uncheck the Show check-box next to the Experiment names.

Fast Exchange Study Dialog

This dialog can be obtained in two ways:

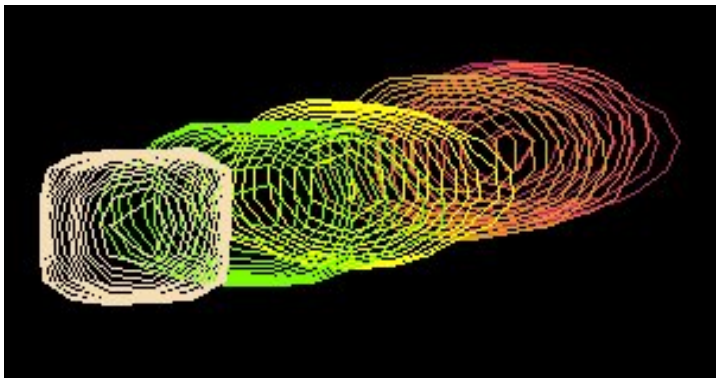
1. Creating new study from New Study Dialog Panel with Fast Exchange Study selected.
2. By clicking on the Edit button on the XippPanel when a Fast Exchange study is selected.



Fast Exchange Study

This dialog defines one Fast Exchange series with 6 ^{15}N-HSQC NMR experiments.

Most of the buttons for the Fast Exchange Study Dialog are the same as described previously. The column Fraction Offset identifies the fraction offset from the first NMR experiment to this experiment. This should be a value between 0.0 and 1.00 which allows vector peak-picking to peak-pick a residue that changes frequency using a single gesture with all peaks sharing same peak-pick ID and label.



Vector peak picking is done by depressing the left (add peak) or right (delete peak) mouse button starting the mouse at one end of the fast exchange set of peaks and releasing the button after dragging the mouse to the opposite end of the set of peaks. If the Fraction Offset is close to correct and the chemical shifts are in fast exchange then Xipp will correctly add a peak in the right place or remove a peak from the right place in each experiment.

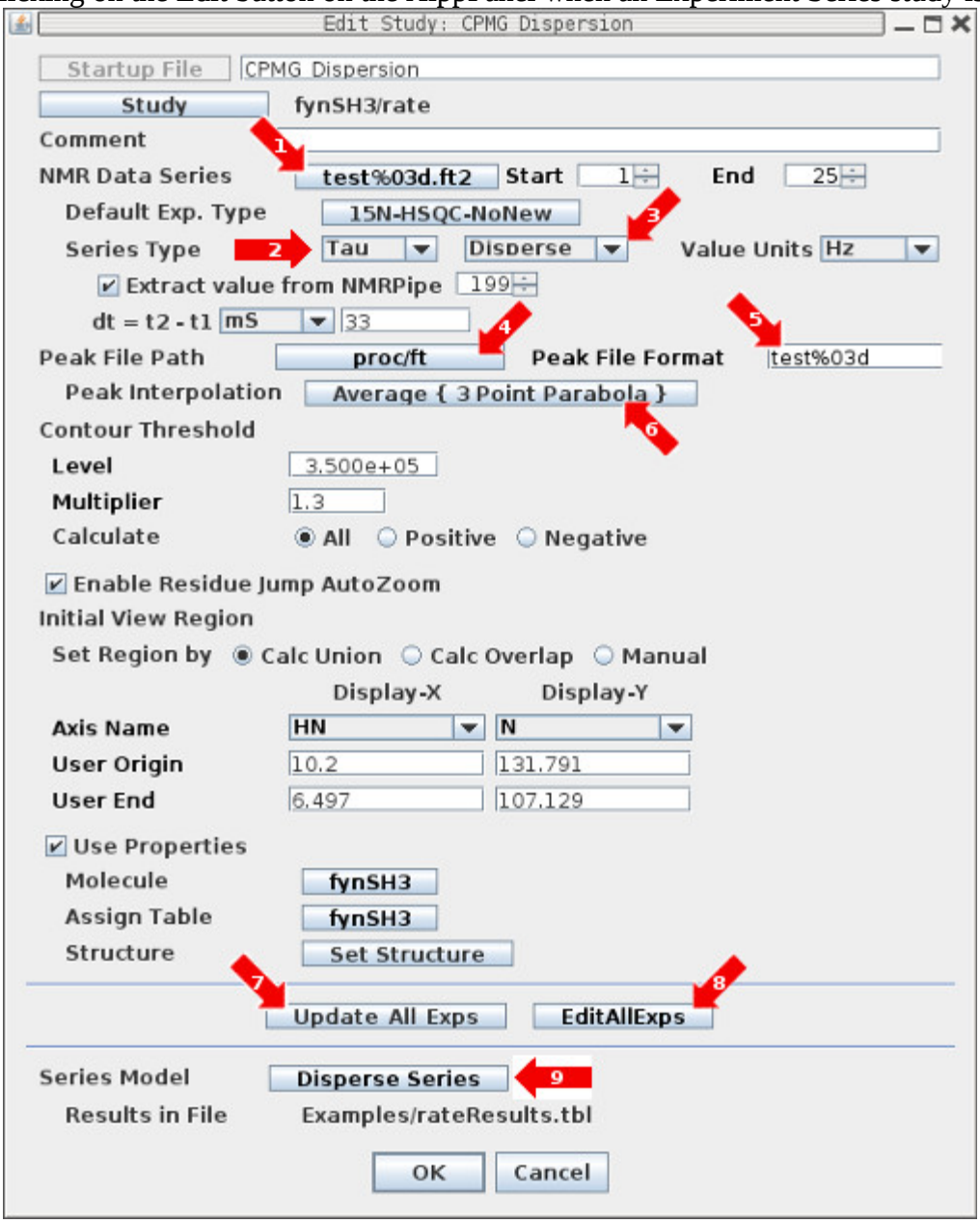
Tip using vector peak picking and moving peaks together is an easy way to copy the assignment label from a reference experiment to all of the experiments involved in the fast exchange.

Clicking OK at the bottom of the Edit Study Dialog will save all of the properties into the file based on the study name, ie fastExchange.xipp in this example.

Experiment Series Study
for CPMG Dispersion

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with type Experiment Series Study.
2. By clicking on the Edit button on the XippPanel when an Experiment Series study is selected.



The Experiment Series Study allows the creation of a variety of Experiment Series based on a series of 2D ^{15}N-HSQC spectra. Shown here is a CPMG Dispersion series with 25 2D ^{15}N-HSQC experiments. Selecting Series Type (2) a Tau and sub-type Disperse makes it a CPMG Dispersion.

Note the text on a button will be red when the properties accessed by that button are not correctly set.

Experiment Series Study
for CPMG Dispersion

This dialog defines one CPMG Dispersion Experiments Series Study with 25 ^{15}N-HSQC NMR experiments.

1: The 'NMR Data Series' button is used to bring up the Series NMR Data File-Set Chooser Dialog to select the series of 2D NMR experiments. Note the file names must include number in sequential order such as test001.ft2, test002.ft2, test003.ft2, . . . test024.ft2 and test025.ft2 so that Xipp can identify the series using a simple name such as test%03d.ft2 which will be used as the text on this button.

2: The Series Type button determines the type of Series. This can be set to Series, Time or Tau.

3: The button next to Series Type is the Series sub-type and its allowed settings depend on the selection for Series Type. For Series only Generic is allowed for sub-type. For Time the sub-type can be Generic, T1, T1p or T2. For Tau the sub-type can be Generic or Disperse. Changing the Series Type and sub-type automatically changes the 'Series Model'.

4: The Peak File Path button brings up a Peak-Pick File chooser to select a directory for the Peak-Pick files. Each 2D experiment will have its own Peak-Pick file. By default this is set to the same directory as the NMR data was located.

5: The Peak File format defines the format for the name for each Peak-Pick file and by default is the same as the file name for the NMR experiments excluding the file extension. The Peak-Pick file names all have .ASG and .PCK as their extension so the Peak-Pick file names will not overwrite the NMR data file names (unless of course you choose to name your experiments test%03d.ASG which would cause the Peak-Pick file to overwrite the NMR Data data file).

6: The 'Peak Interpolation' button brings up the Peak Pick Options dialog to select type of interpolation on Initial Experiment and Ensuing Exps.

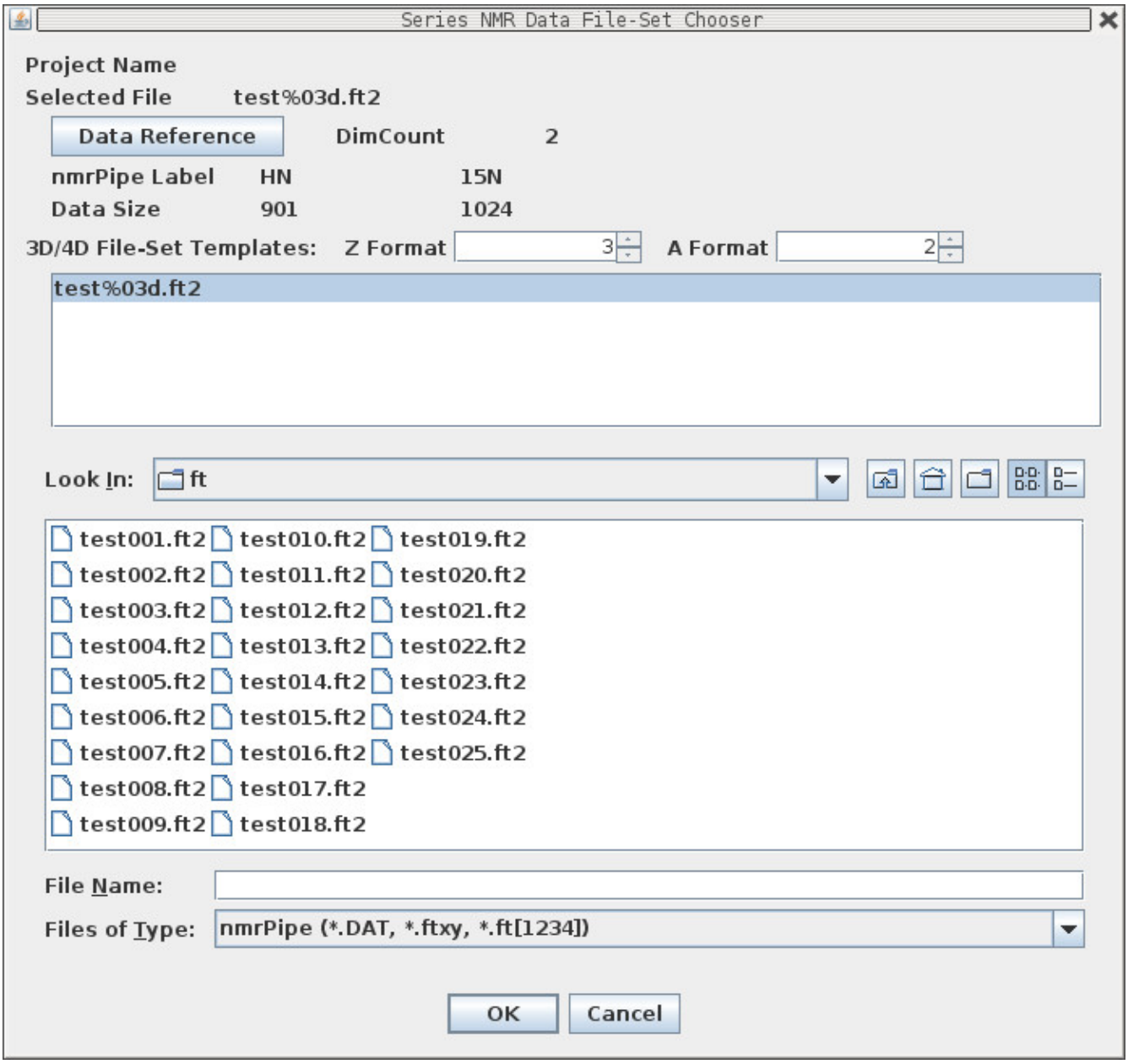
7: The 'Update All Exps' button will copy the properties on this dialog to each 2D Experiment. When the Study is first created and the OK button is clicked all 2D experiments are automatically updated. After the Study has been created and saved and when it is edited any changes to Peak File Path/Format, Contour Threshold, Initial View Region and Use Properties (Molecules & Assign Table) will not automatically update to each 2D NMR Experiment unless the Update All Exps is clicked.

8: The 'Edit All Exps' button brings up the Edit Experiment Series dialog that allows setting properties for individual Exps. This should not be needed under normal situations, but exists to provide the flexibility to set properties differently for individual experiments. The Edit Experiment Series dialog also provides a way to set and confirm the Tau value for each experiment if this was not set when the data was processed by NMRPipe.

9: The 'Series Model' button brings up the Model dialog which allows setting the Results files and formatting.

Series NMR Data File-Set Chooser

This dialog is obtained by clicking the NMR Data Series button from the Experiments Series Dialog.

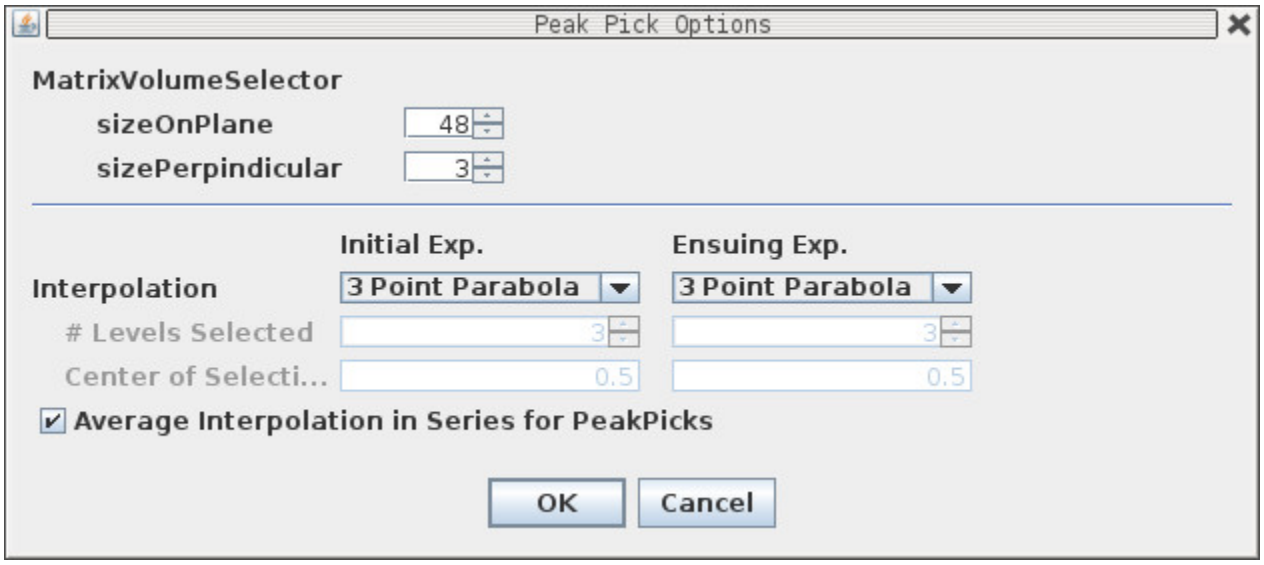


This Dialog is very similar to the NMR Data File Chooser.

When the NMRPipe file or file set is selected the DimCount, nmrPipe Label and Data Size are updated from NMRPipe header.

Peak Pick Options Dialog

This dialog is obtained by clicking the Peak Interpolation button from the Experiments Series Dialog.



The default options are usually good for most NMR Experiments.

The MatrixVolumeSelector defines the number of points to read in around the position of the mouse when doing peak picking. For highly zero-filled data it might be necessary to increase sizeOnPlane.

There are three type of interpolation:

3 Point Parabola

Start at mouse position and go up the steepest gradient to find the local extrema. Fit the top 3 points to a parabola and report the top of the parabola as the peak position for each axis.

Contour Average

Start at mouse position and go up the steepest gradient to find the local extrema. Average the X,Y position of contours that encircle local extrema at selected percent of peak height to define peak position on contoured X, Y plane. This usually works best with well resolved peaks and high zero-filling.

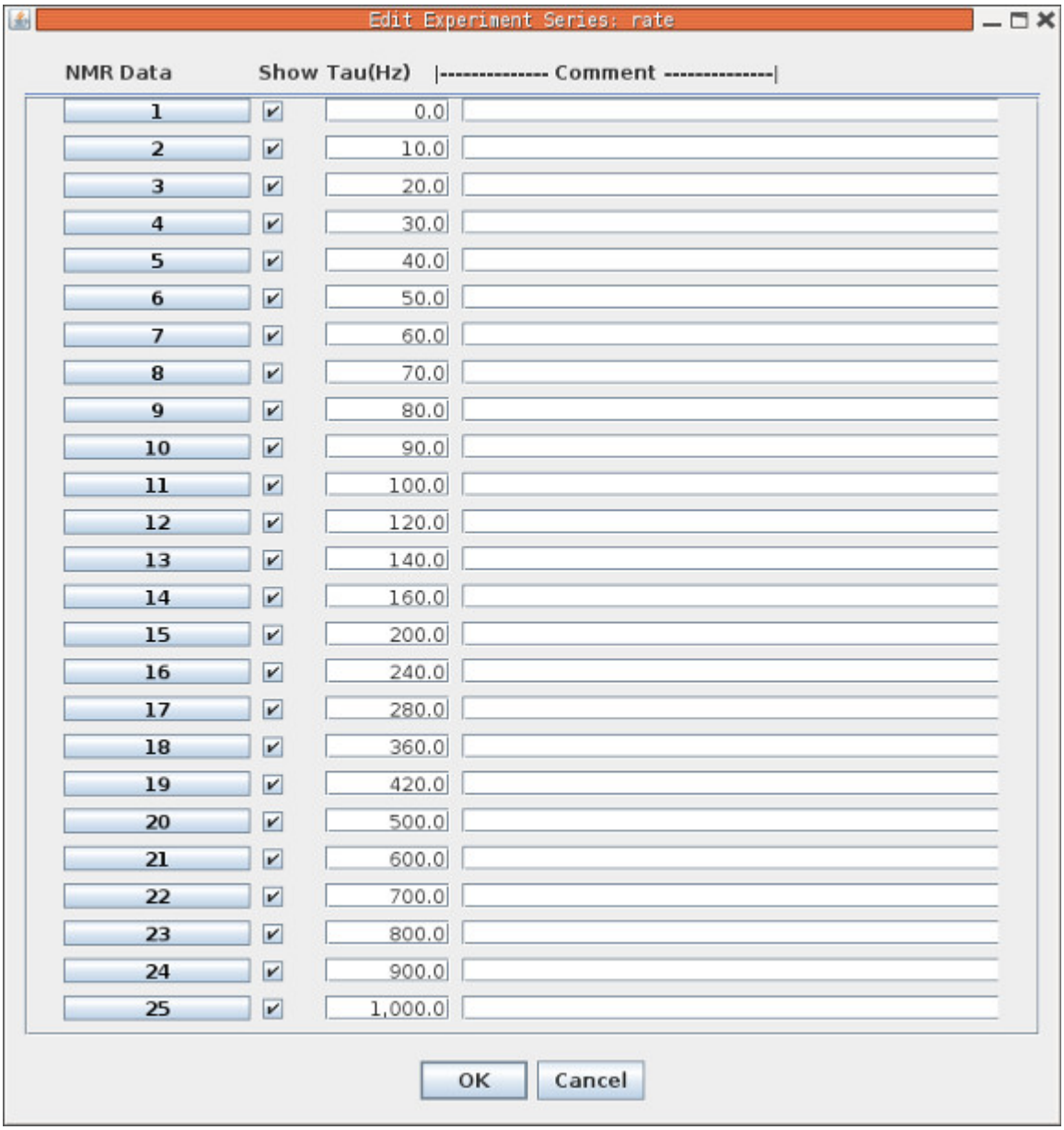
Same Position

Use the same X, Y PPM position as determined from previous Exp. This can only be set for Ensuing Exp., it can not be used for Initial Exp.

When the Average Interpolation in Series for PeakPicks is checked the Xipp will average the X, Y value obtained from Initial and Ensuing Exp and use that point in all Experiments to get the intensity from each Experiment in the series.

Edit Experiment Series

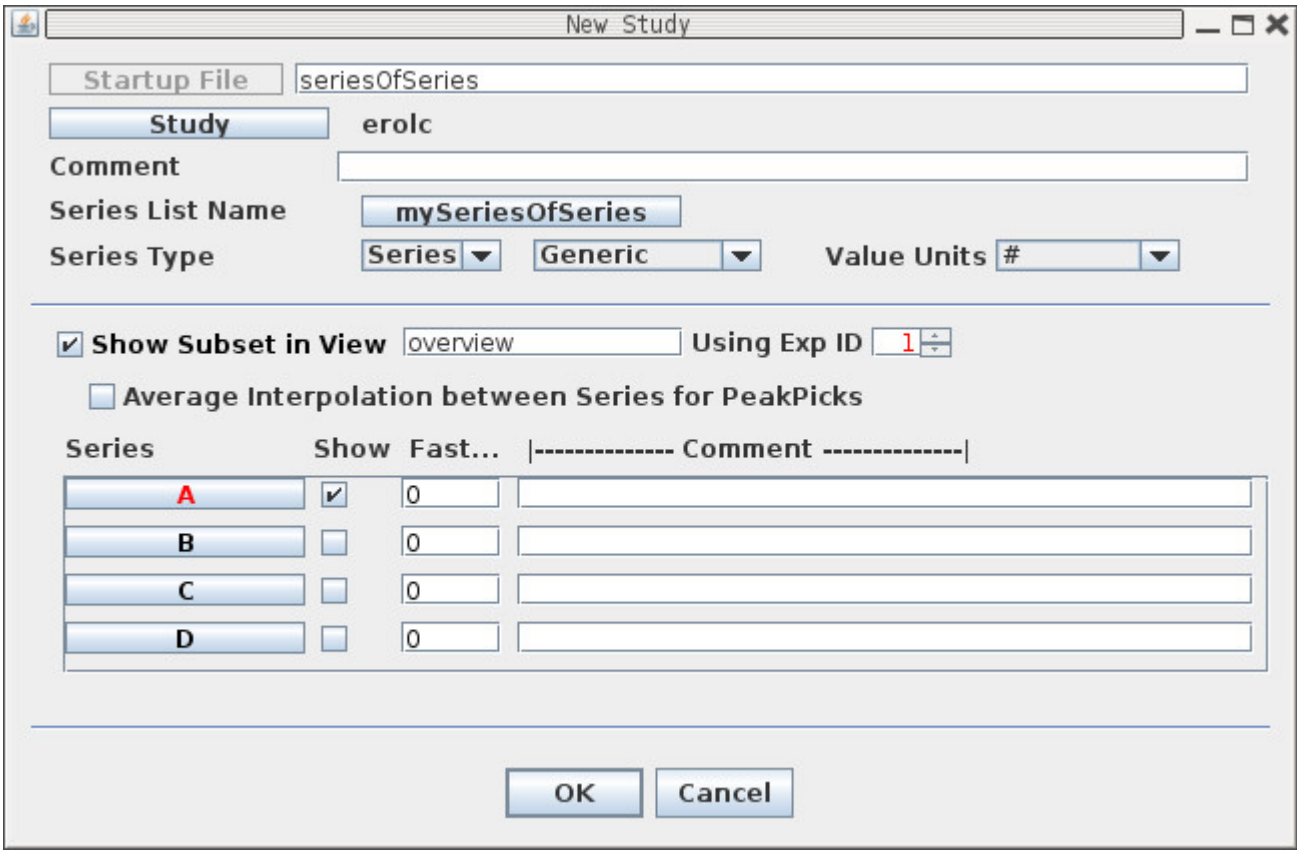
This dialog is obtained by clicking the Edit All Exps button from the Experiments Series Dialog.



Clicking one of the NMR Data buttons which are labeled with the exp number brings up the Edit Experiment dialog for that experiment. Note the text on the buttons will be red when the properties are not correctly set.

The Tau value is initially set from NMRPipe file header location 199 with experiment specific value. In the CPMG Disperse shown here the CPMG field strength in Hz is shown for each experiment.

Series of Series Study



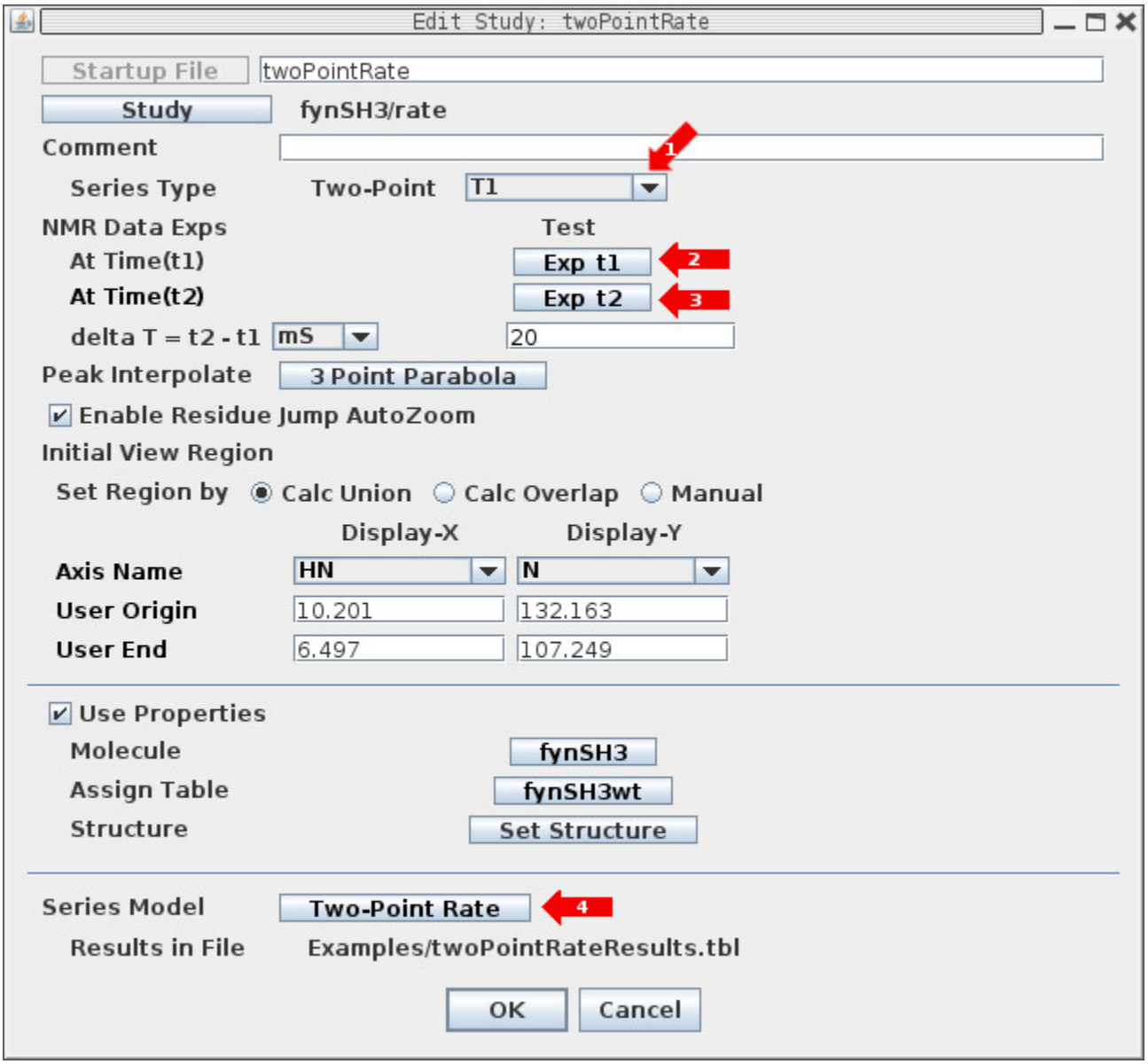
The Series of Series is used to show multiple Experiment Series and create an overview displaying the first exp from each series. Currently, the Series of Series can not show Multi-Point PRE or Multi-Point Delta Rate Series. I do not have a good example data-set to demonstrate Series of Series.

The Series Type and sub-type options are used only to initialize a new Experiment Series. Changing Series Type or sub-type will not change the type or sub-type of an existing Experiment Series.

Click the button under Series, ie A, to define a single Experiment Series. Note the text on the button will be red when the properties are not correctly set which will always be true for A when the Study is first created.

The column labeled Fast. . . can be used to set Fraction Offset for each Exp Series so that the Subset View named overview will look like a simple Fast-Exchange.

Two-Point Rate Study



1: The Series Type is fixed to Two-Point and the Sub-Type can be set to T1, T2 and T1p. Changing the Sub-Type has no effect at this time.

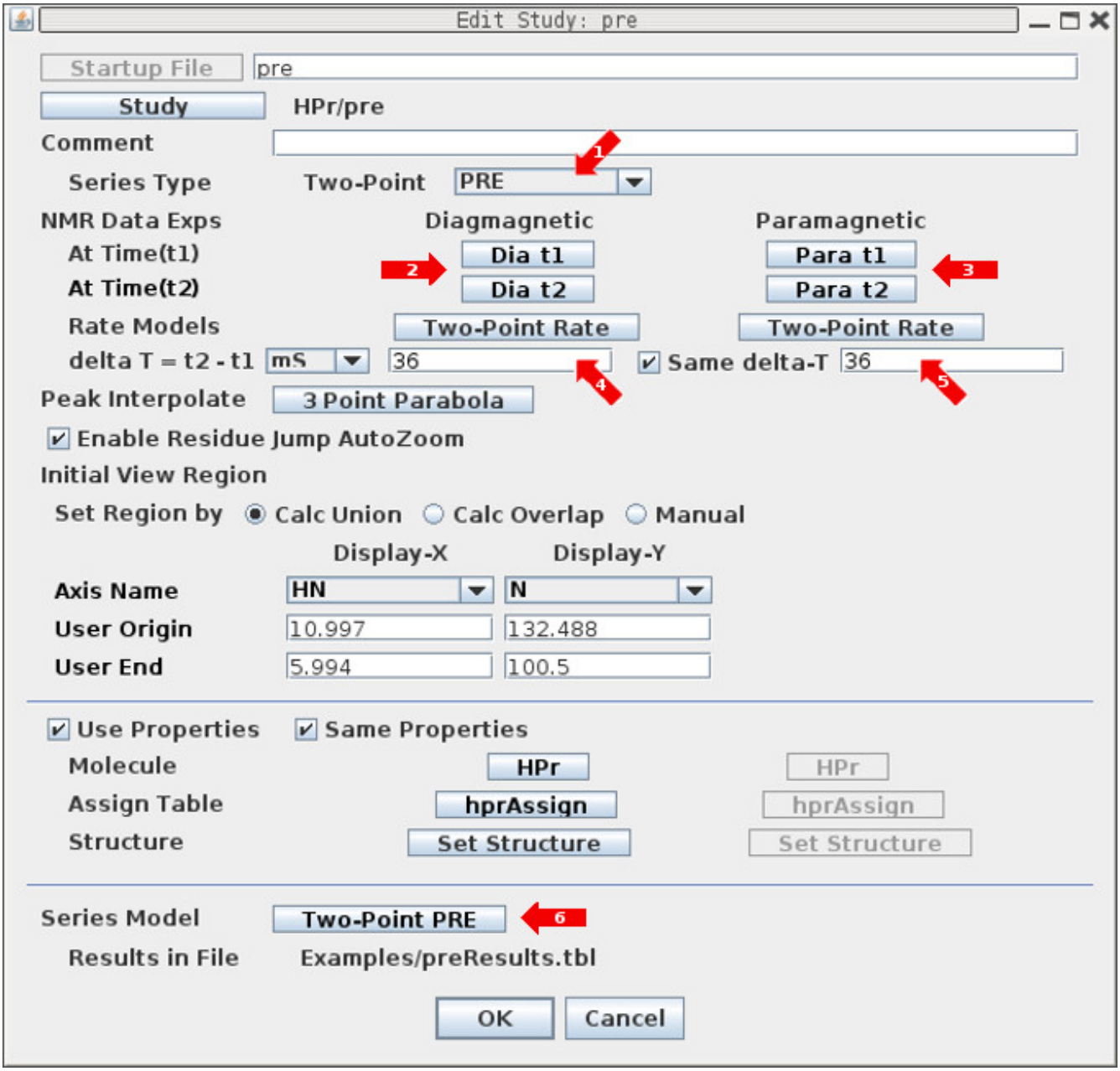
2: Click button Exp_t1 to bring up the Edit Experiment Dialog in order to define the location and properties of the 2D ^{15}N HSQC NMR experiment at the first time point (ie t1).

3: Click button Exp_t2 to bring up the Edit Experiment Dialog in order to define the location and properties of the 2D ^{15}N HSQC NMR experiment at the second time point (ie t2). Note the text on the buttons will be red when the properties are not correctly set.

4: Click Two-Point Rate button to change Series Model properties which include location of Results File and formatting specification.

Two-Point PRE Study

The Two-Point PRE and Two-Point Delta Rate use the same dialog and differ by selecting PRE or Delta-R2 in option 1 and having different Series Model in 6.



Two-Point PRE Study

1: The Series Type is fixed to Two-Point and the Sub-Type can be set to PRE or Delta-R2. Changing the Sub-Type has no effect at this time except to change the Series Model and Results file name.

2: Click buttons Dia_t1 and Dia_t2 to bring up the Experiment Dialog at time t1 or t2 respectively to define the file names and properties of the 2D ^{15}N HSQC NMR experiments for the Diamagnetic experiments. Note the text on the buttons will be red when the properties are not correctly set.

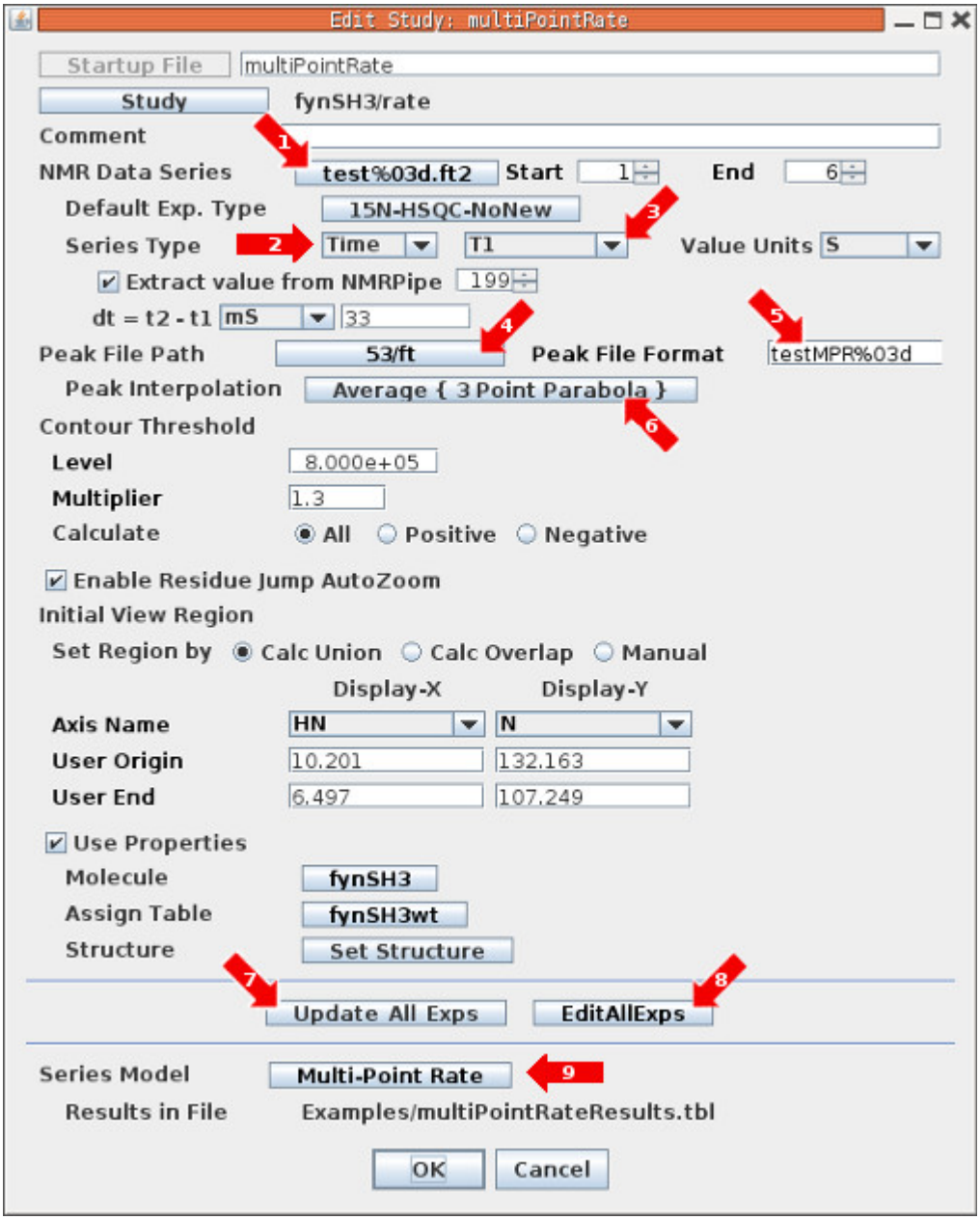
3: Click buttons Para_t1 and Para_t2 to bring up the Experiment Dialog at time t1 or t2 respectively to define the file names and properties of the 2D ^{15}N HSQC NMR experiments for the Paramagnetic experiments. Note the text on the buttons will be red when the properties are not correctly set.

4: Click Two-Point Rate button to change Series Model properties which include location of Results File and formatting specification.

Multi-Point Rate Study

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with type Multi-Point Rate Study.
2. By clicking on the Edit button on the XippPanel when a Multi-Point Rate study is selected.



Multi-Point Rate Study

This dialog defines one Multi-Point Rate Study with 6 ^{15}N-HSQC NMR experiments. The dialog is the same as used for CPMG Dispersion.

1: The 'NMR Data Series' button is used to bring up the Series NMR Data File-Set Chooser Dialog to select the series of 2D NMR experiments. Note the file names must include a number in sequential order such as test001.ft2, test002.ft2, test003.ft2, test004.ft2, test005.ft2 and test006.ft2 so that Xipp can identify the series using a simple name such as test%03d.ft2 which is used as the text on this button.

2: The Series Type button determines the type of Series. This can be set to Series, Time or Tau.

3: The button next to Series Type is the sub-type and its allowed settings depend on the selection for Series Type. For Series only Generic is allowed for sub-type. For Time the sub-type can be Generic, T1, T1p or T2. For Tau the sub-type can be Generic or Disperse. Changing the Series Type and sub-type automatically changes the 'Series Model'.

4: The Peak File Path button brings up a Peak-Pick File chooser to select a directory for the Peak-Pick files. Each 2D experiment will have its own Peak-Pick file. By default this is set to the same directory as the NMR data was located.

5: The Peak File format defines the format for the name for each Peak-Pick file and by default is the same as the file name for the NMR experiments excluding the suffix. The Peak-Pick file names all have .ASG and .PCK as their suffix so the Peak-Pick file names will not overwrite the NMR data file names (unless of course you choose to name your experiments test%03d.ASG which would cause the Peak-Pick file to overwrite the NMR Data data file).

6: The 'Peak Interpolation' button brings up the Peak Pick Options dialog to select type of interpolation on Initial Experiment and Ensuing Exps.

7: The 'Update All Exps' button will copy the properties on this dialog to each 2D Experiment. When the Study is first created and the OK button is clicked all 2D experiments are automatically updated. After the Study has been created and saved and when it is edited any changes to Peak File Path/Format, Contour Threshold, Initial View Region and Use Properties (Molecules & Assign Table) will not automatically update to each 2D NMR Experiment unless the Update All Exps is clicked.

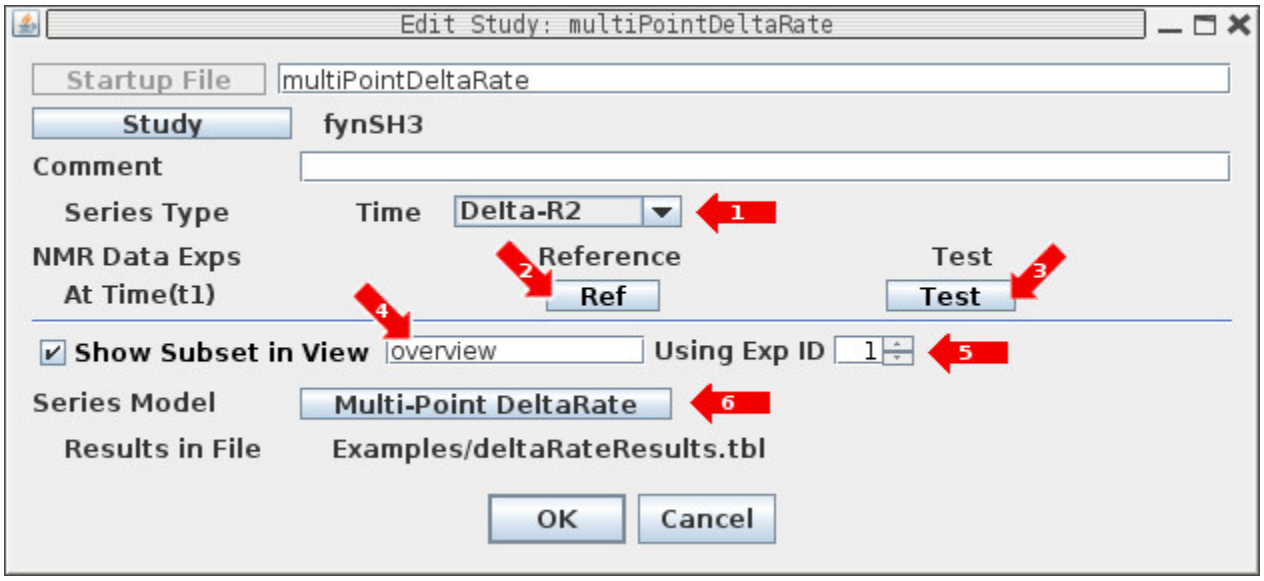
8: The 'Edit All Exps' button brings up the Edit Experiment Series dialog that allows setting properties for individual Exps. This should not be needed under normal situations, but exists to provide the flexibility to set properties differently for individual experiments. The Edit Experiment Series dialog also provides a way to set and confirm the Tau value for each experiment if this was not set when the data was processed by NMRPipe.

9: The 'Series Model' button brings up the Model dialog which allows setting the Results files and formatting.

Multi-Point Delta Rate Study

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with type Multi-Point Delta Rate Study.
2. By clicking on the Edit button on the XippPanel when a Multi-Point Delta Rate study is selected.



1: The Series Type is fixed to Time and the Sub-Type can be set to PRE or Delta-R2.

2: Click button Ref to bring up the Multi-Point Rate Study Dialog for the Reference Experiment Series.

3: Click button Test to bring up the Multi-Point Rate Study Dialog for the Test Experiment Series.

4: The default name of the Subset view overview which can be changed in this text field.

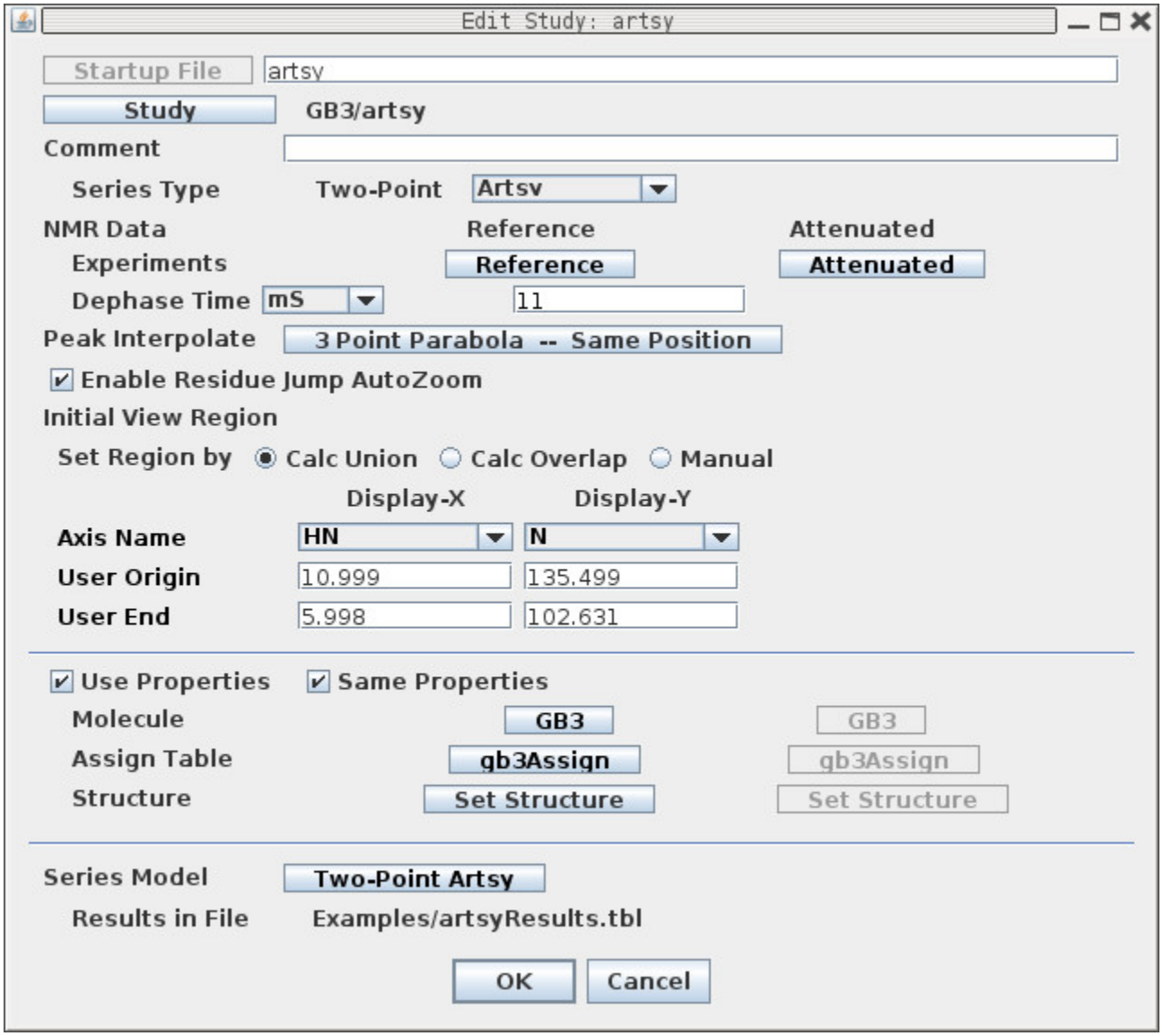
5: The Exp-ID from Reference and Test that are overlaid in the Subset View is defined by 'Using Exp ID'

6: Click Multi-Point DeltaRate button to change Series Model properties which include location of Results File and formatting specification.

ARTSY Study Dialog

Reference for ARTSY:

N.C. Fitzkee and A. Bax J. Biol NMR (2010)
Facile measurement of 1H-15N residual dipolar couplings in larger perdeuterated proteins.
http://dx.doi.org/10.1007/s10858-010-9441-9



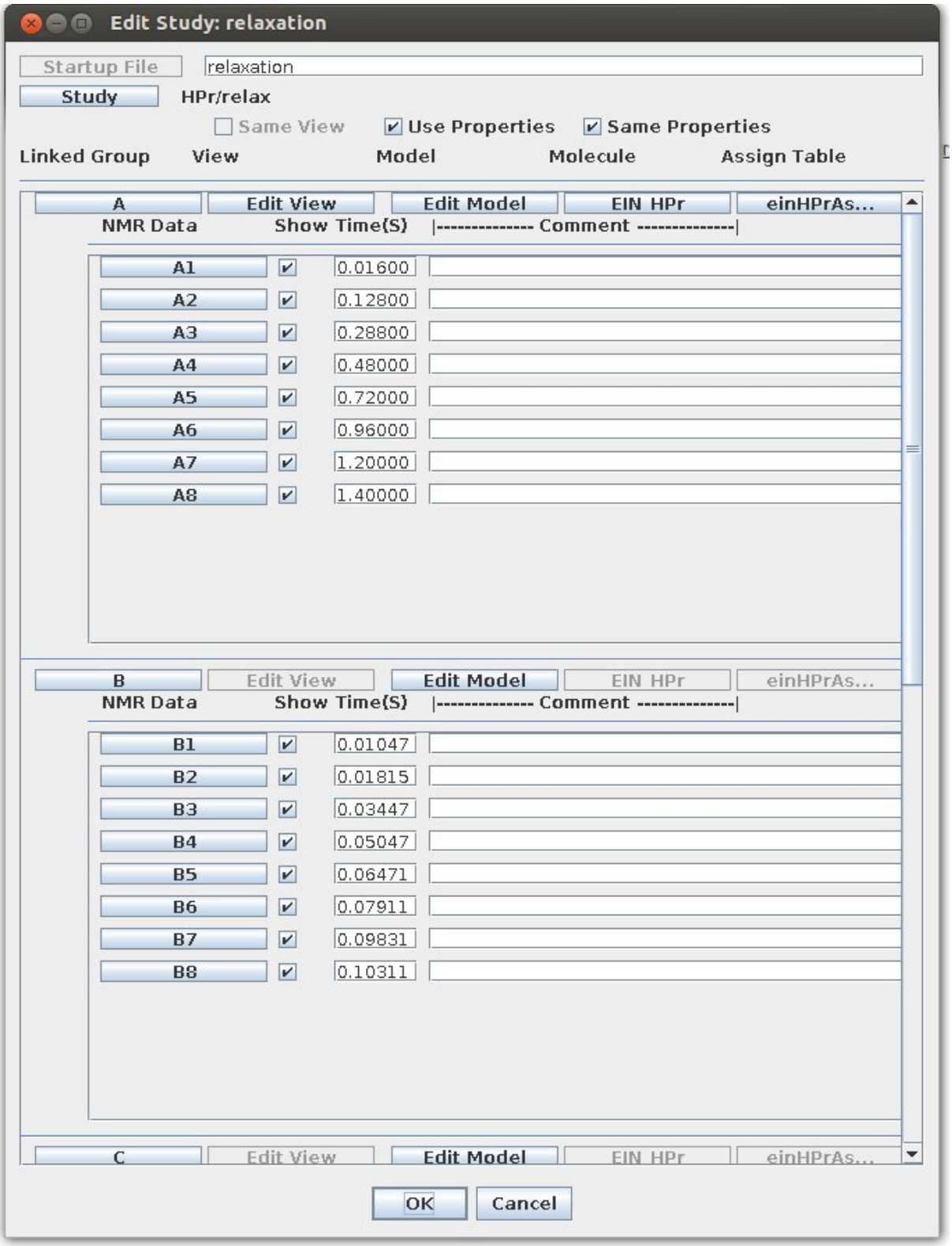
Most of the buttons for the ARTSY Study Dialog are the same as described previously for Two-Point Studies. The Dephase Time(mS) identifies the relaxation time for each experiment in user selectable mS or S.

By default the Peak Interp for the Attenuated NMR experiment is set to 'Same Position' which uses the same X,Y data point for the Attenuated data as was interpolated in the Reference NMR experiment. Note 'Same Position' can be used in a series after the first Exp.

Old Relaxation (T1,T2) Study Dialog

This dialog can be obtained in two ways:

1. Creating new study from New Study Dialog Panel with Relaxation (T1, T2) Study selected.
2. By clicking on the Edit button on the XippPanel when a Relaxation (T1, T2 study is selected.



Old Relaxation (T1, T2) Dialog

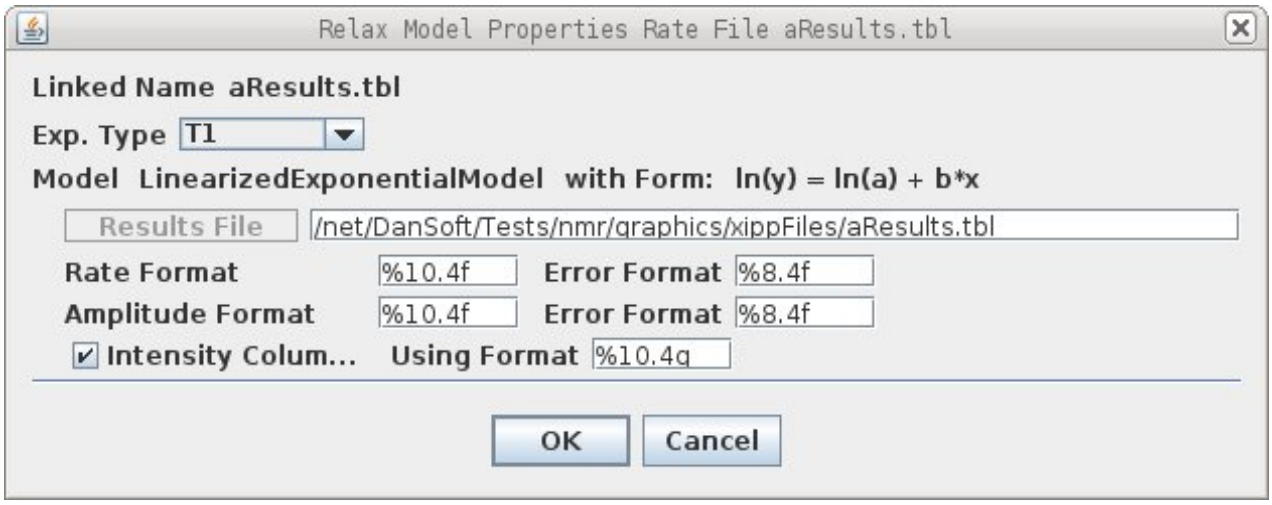
This dialog I sthe old way of analysing T1 and T2 experiments and is being deprecated. This defines 2 sets of T1 and T2 (or T1rho) with 8 NMR experiments each. In order to increase the number of NMR experiments or increase the number of sets of T1 or T2 groups you need to edit the Python file configTree.py which by default is installed at ~/Xipp/v1/lib/nmr The part that needs to change is about 100 lines after: 'class RelaxStudyExpNode'. Look for the following:

```
self.createExpNode( "relax",    "A",      "15N-HSQC", "A1"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A2"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A3"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A4"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A5"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A6"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A7"    ),
self.createExpNode( "relax",    "A",      "15N-HSQC", "A8"    ),
```

Each line above identifies a separate T1 experiment. The last argument to creatExpNode is the name of the NMR experiement and must be unique. To increase the number of Experiments add new lines with unique NMR data names. Note this is Python so the syntax must be correct.

Most of the buttons for the Relaxation Study Dialog are the same as described previously. The column Time(S) identifies the relaxation time for each experiment in seconds.

The Edit Model button brings up the Relaxation Model Properties Dialog:



Changing Exp. Type only changes a label in the output. The Exp. Type is not important for fitting the data to the LinearizedExponentialModel.

Clicking OK at the bottom of the Edit Study Dialog will save all of the properties into the file based on the study name, ie relaxation.xipp in this example.