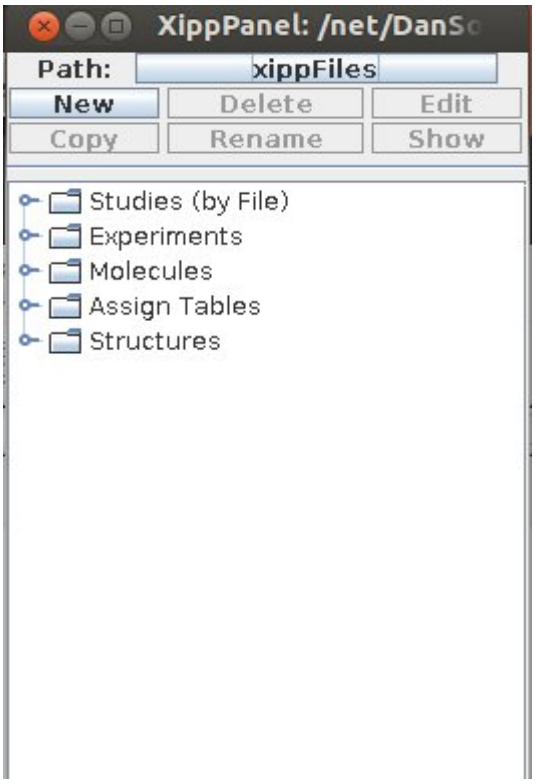
Starting Xipp on Linux
from a terminal window

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.

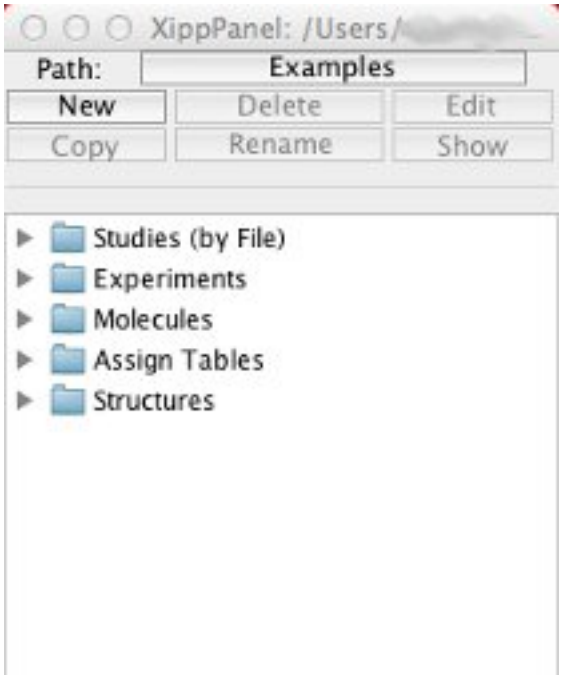
xippOutput.log

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.

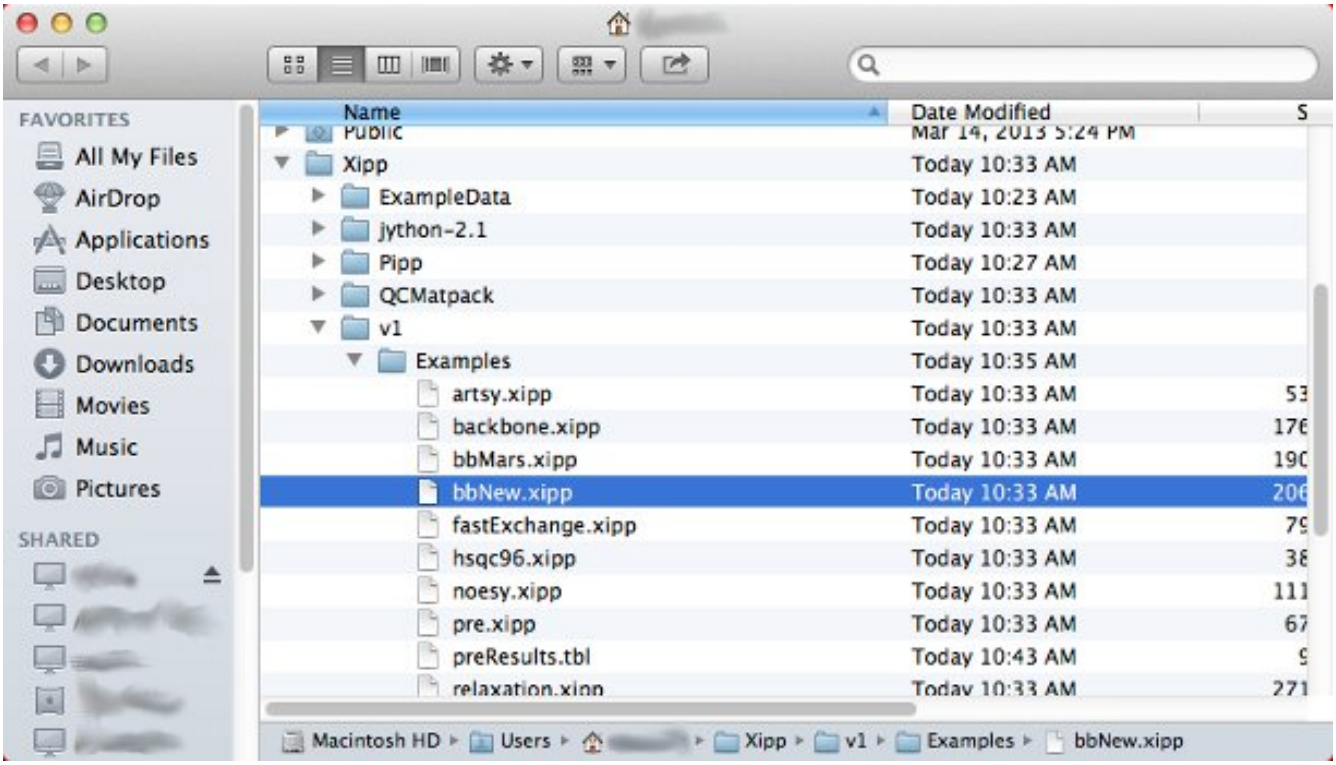
xipp backbone.xipp

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

xipp startXipp.py

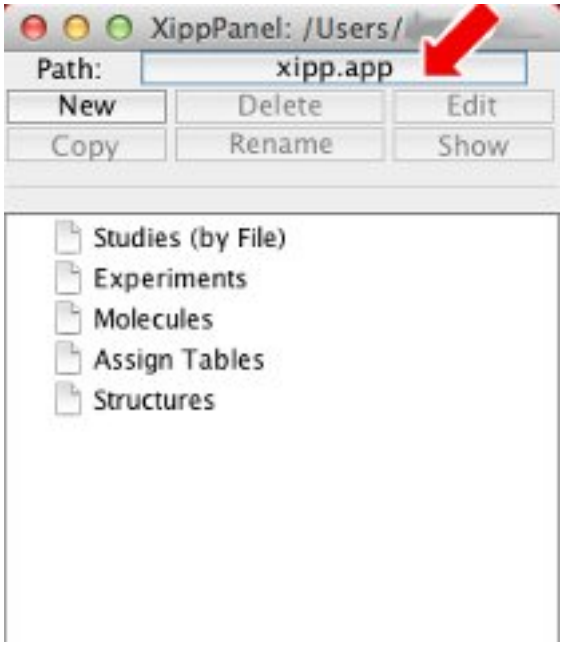
Start Xipp from Python file by creating and initializing DataServer and GUI Objects.
During development new Java Objects are first implemented by making changes to the startXipp.py and the Python library before implementing in XippPanel.

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.

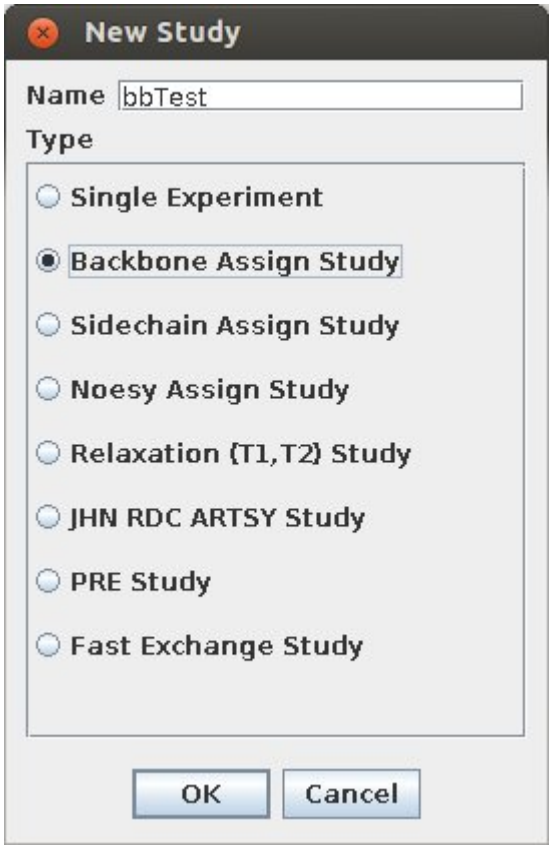
xippOutput.log

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.

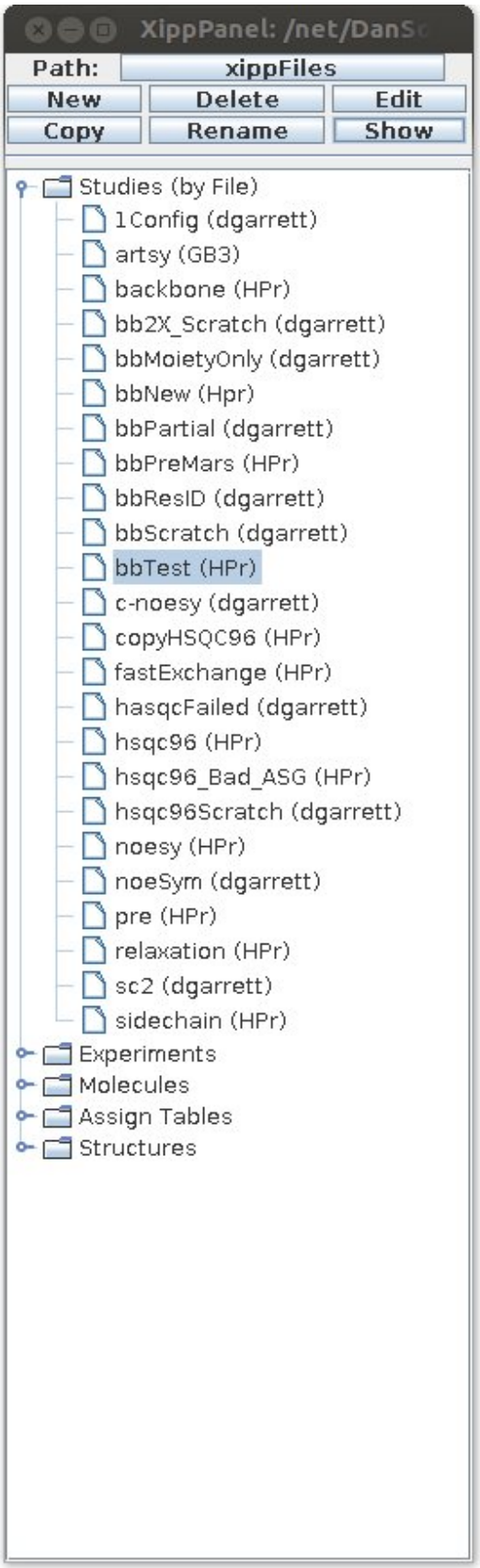


Must enter unique Name and select type of Study to create and show study specific Panel.

The name for a new study will be used to create a file in directory as given by Path in XippPanel that will define the properties of this study.

In this example the file 'bbTest.xipp' will get created for a Backbone Assign Study.

Editing Study Properties



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

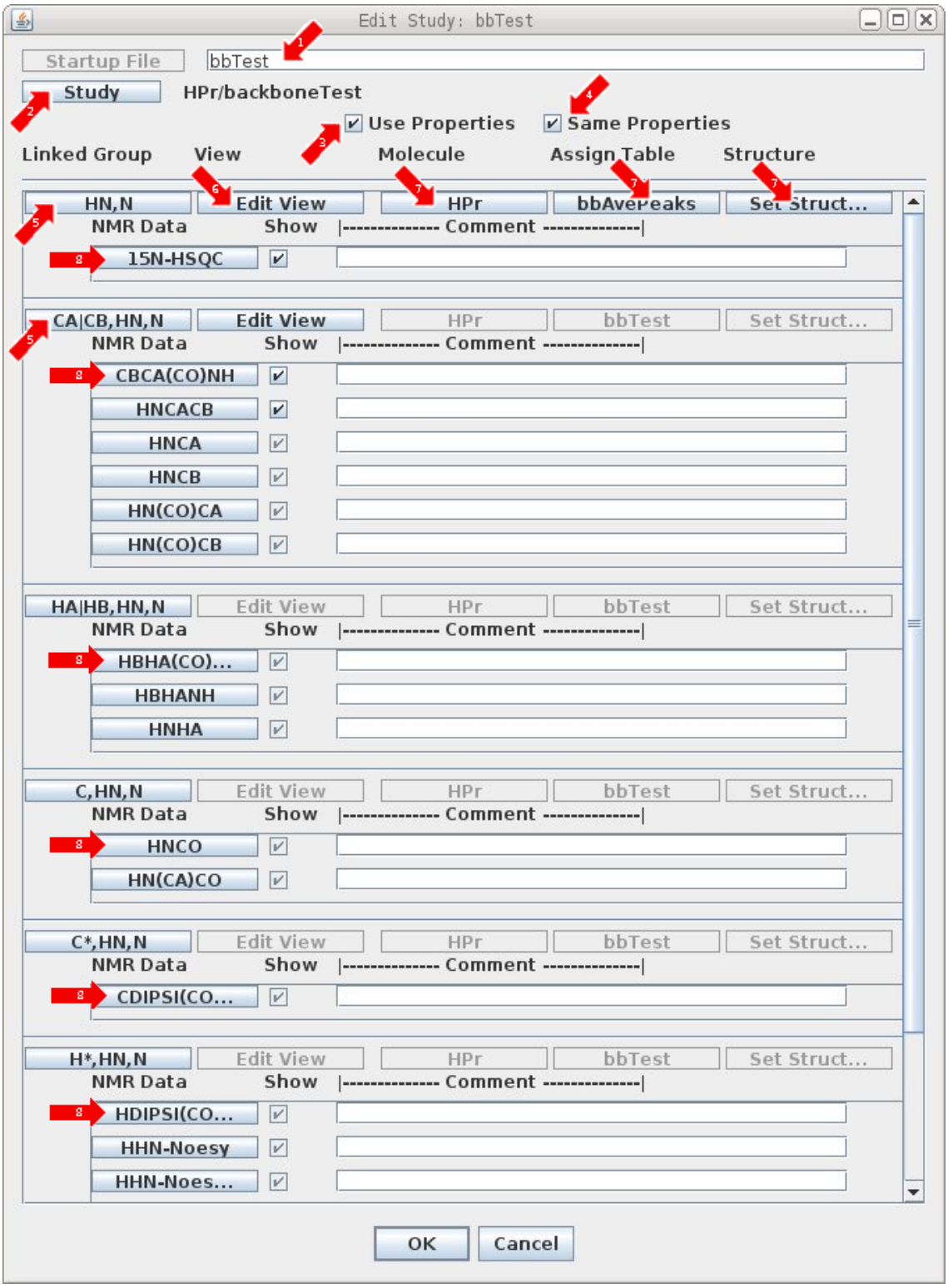
Currently there are 8 types of Studies:

- Single Experiment
  - Any 2D or 3D experiment.
- Backbone Assign Study
  - Links groups of backbone assign experiments based on ability to overlay spectra.
- Sidechain Assign Study
  - Links groups of sidechain assign experiments based on ability to overlay spectra.
- Noesy Assign Study
  - Links groups of NOE experiments based on ability to overlay spectra.
- Relaxation (T1,T2) Study
  - Creates up to 4 sets of linked groups for T1 and T2 relaxation. Uses Linearized Exponential Model to estimate rate.
- JHN RDC ARTSY Study
  - Defines Reference and Attenuated to calculate ARTSY coupling constant for each residue.
- PRE Study
  - Defines Dia_t1, Para_t1, Dia_t2 and Para_t2 to calculate 2 point PRE R2.
- 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.

Edit Study: Backbone Assign Dialog

This dialog can be obtained in two ways:

1. Creating a new study by clicking OK on New Study Dialog Panel.
2. By clicking on the Edit button on the XippPanel when a study is selected.



Edit Study: Backbone Assign Dialog

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. Clicking the old study name brings 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 all of the Linked Groups 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.

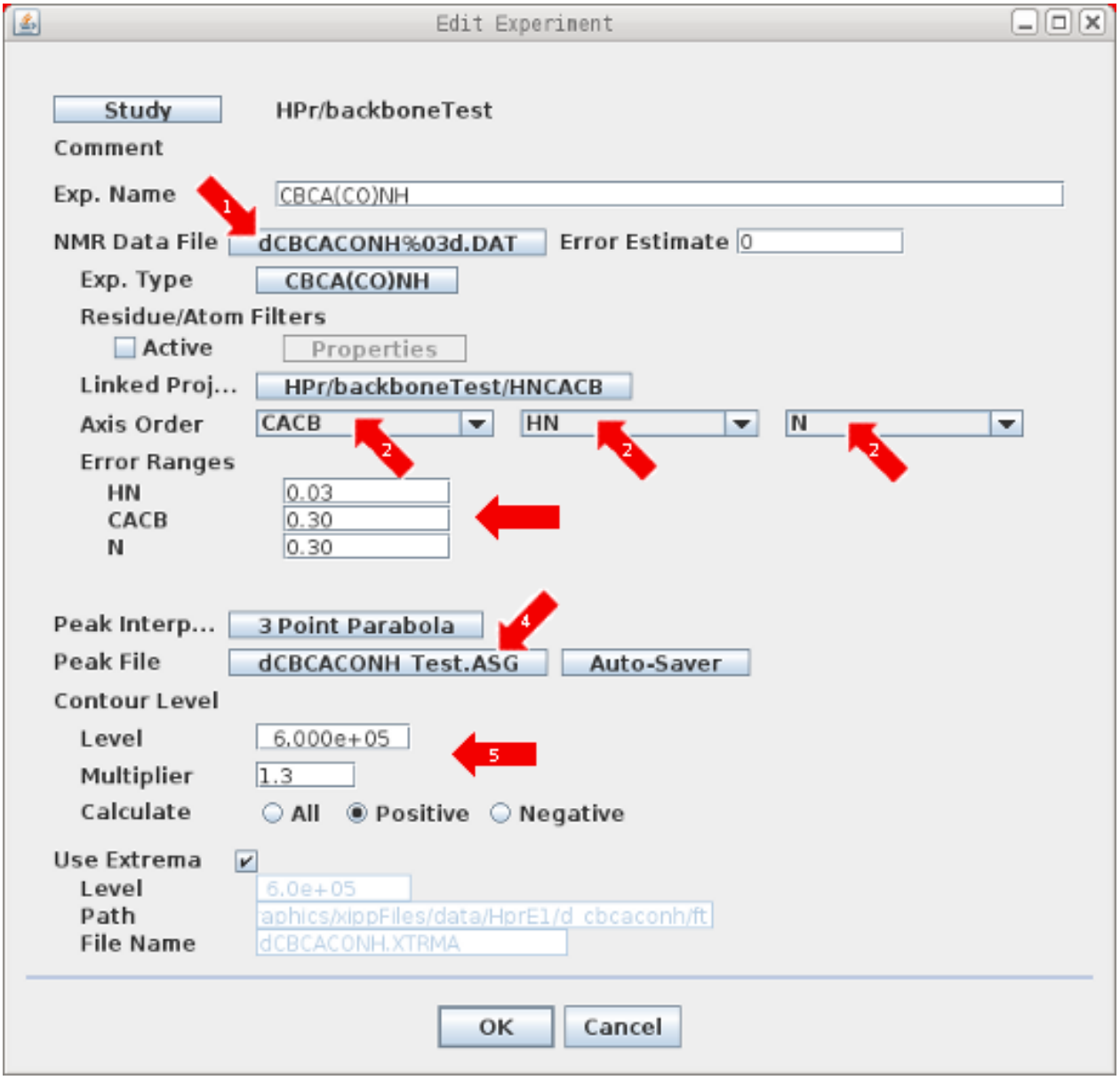
7: The Molecule, Assign Table and Structure buttons for each linked group bring up the Select/Create Dialog for Molecule, Assign Table and Structure respectively.

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.

NMR Data Experiment Dialog

This dialog is obtained by clicking the CBCA(CO)NH button on the Edit Study: Backbone Assign Dialog.

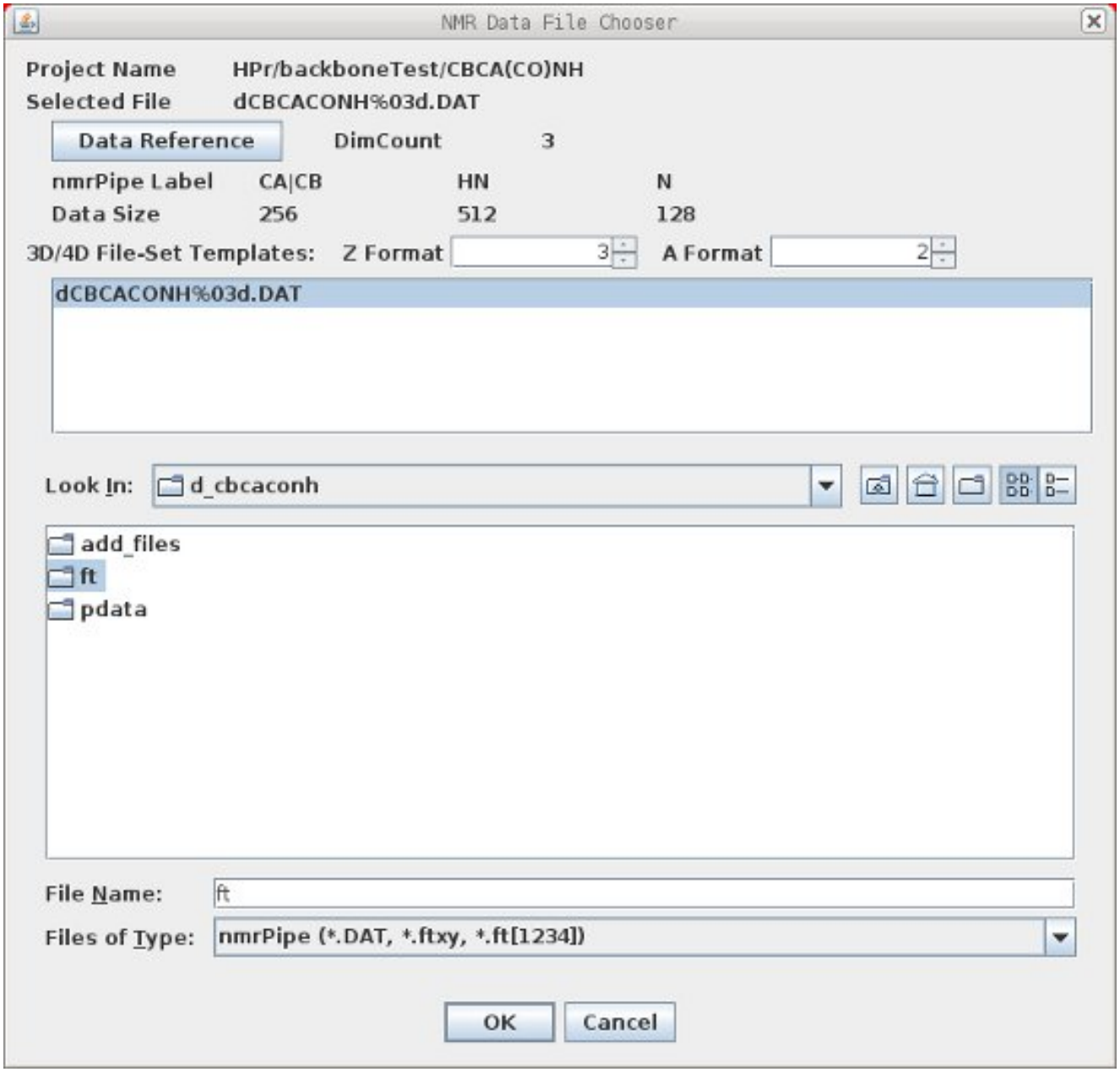


Set/Check Properties: NMR Data File, Axis Order, Peak File and Contour Level

Must set (1) NMR Data File, (2) ensure that Axis Order and (3) Error Ranges are OK. The Axis Order is the order of the Axis (ie X, Y, Z) and is set when the NMR Data File is selected using gyromagnetic ratio of atom types and the carrier frequency defined in NMRPipe header for each axis. Axis Order for identical atom types can not be distinguished and must be set manually. (4) Peak File is set to a default value when NMR Data File is set. Click Peak File button if your want to change it. The (5) Contour Level is the starting level used in Xipp.

NMR Data File Chooser

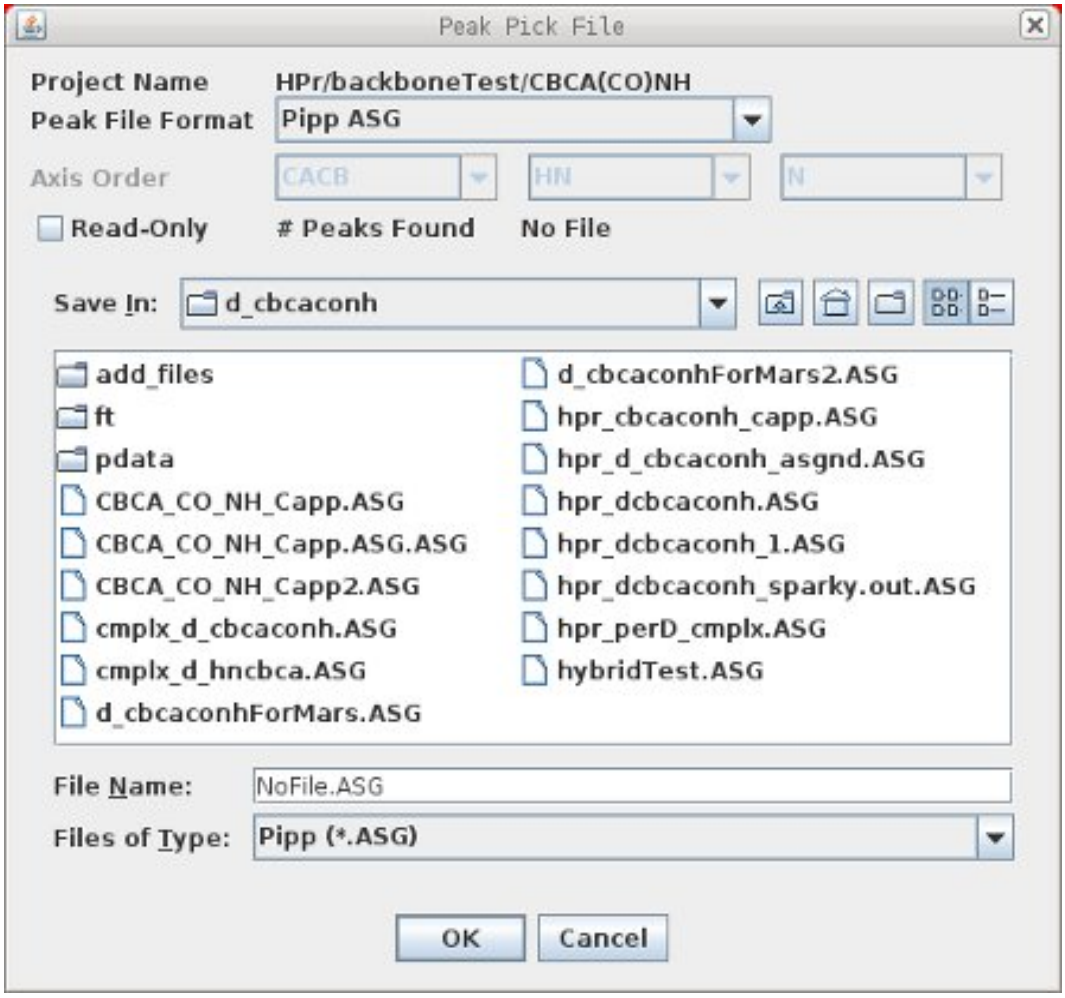
This dialog is obtained by clicking the NMR Data File button from the NMR Data Experiment Dialog.



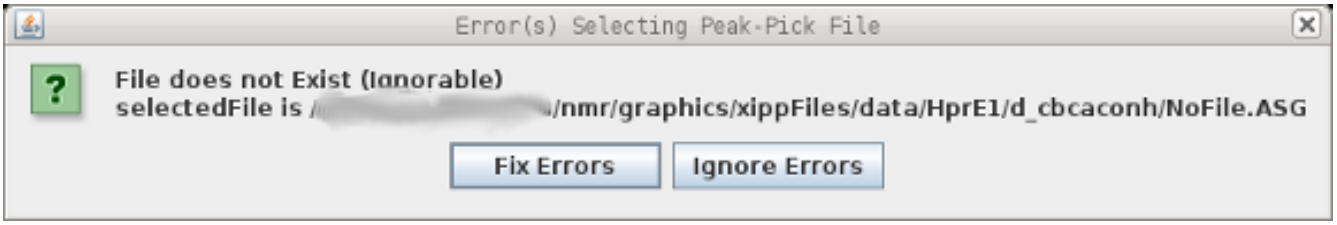
When the NMRPipe file or file set is selected the DimCount, nmrPipe Label and Data Size are updated from NMRPipe header.

Peak Pick File Chooser

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



If the file does not exist the following Error message will appear after clicking OK:

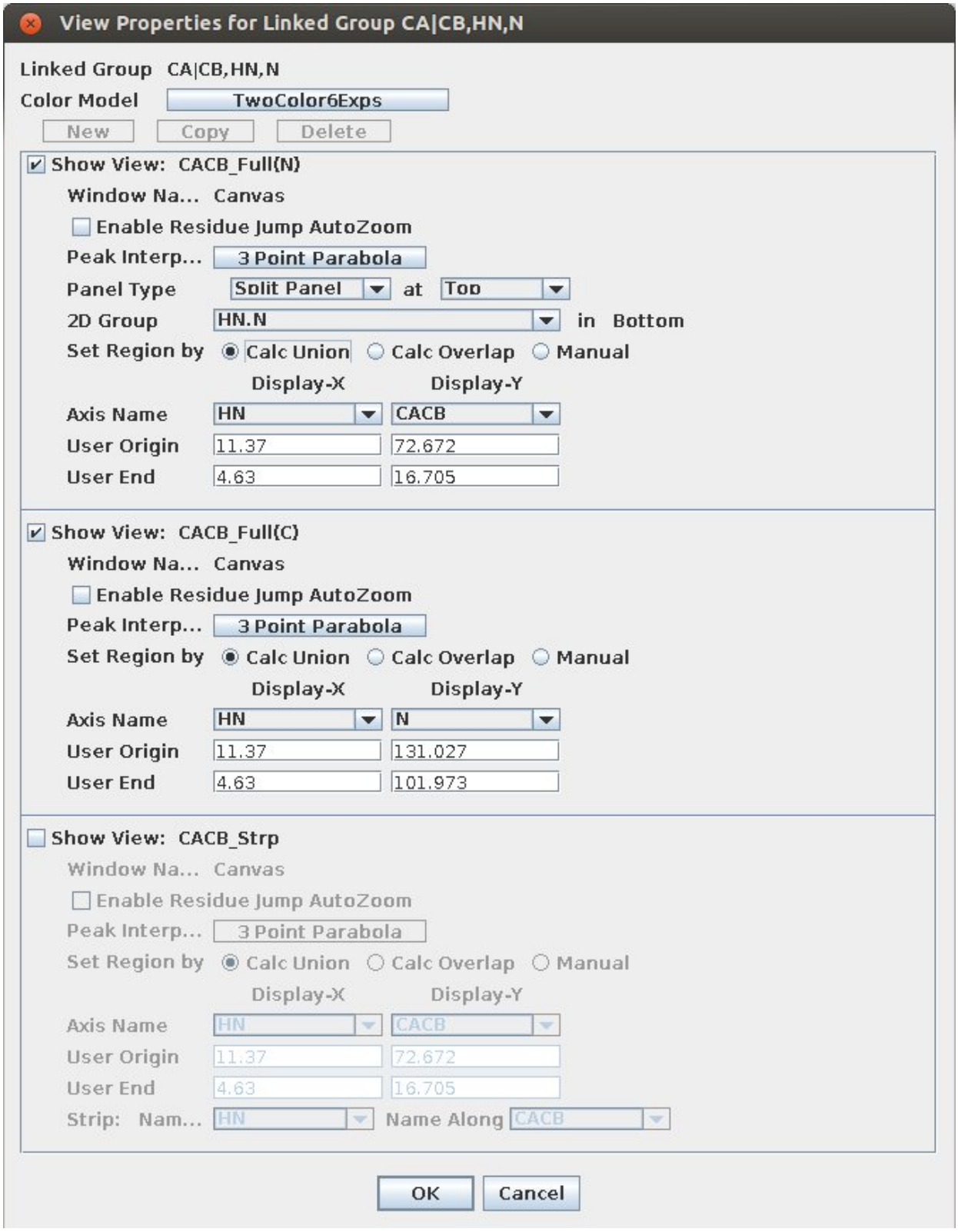


Click Fix Errors to re-show the Peak File Chooser Panel to select an existing file.

Click Ignore Errors to create a new Peak Pick file when Xipp shows this study.

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.

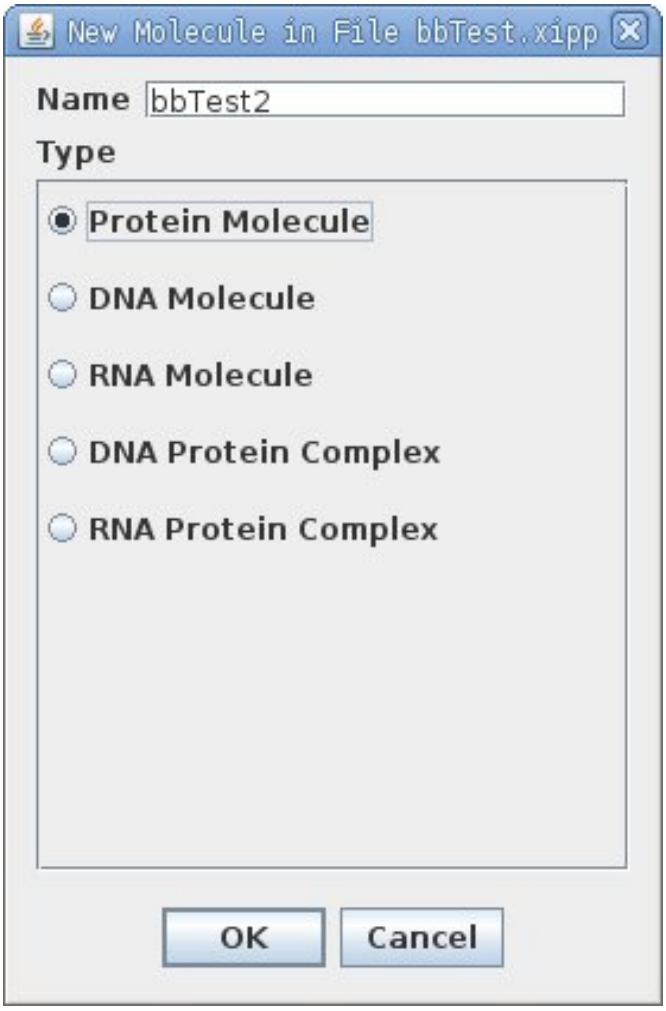
Each molecule name must be unique within its own study, but the same molecule name can be used in different studies.

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

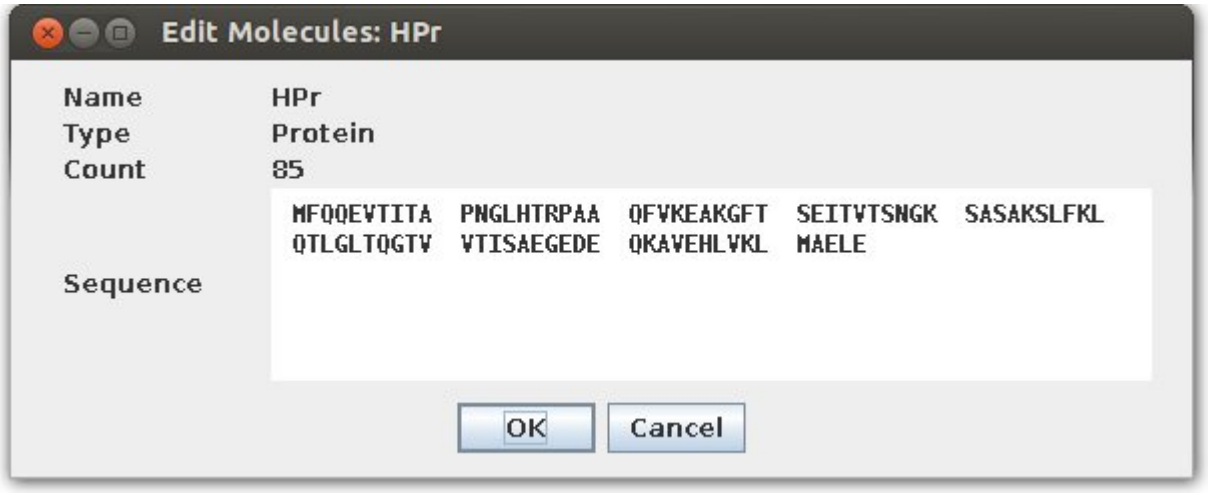
This dialog is obtained by clicking on the New button from the Select/Create Molecule Dialog.
The Name for the molecule must be unique within this study but can be the same name of a molecule used in another study.



Edit Molecules Dialog

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.

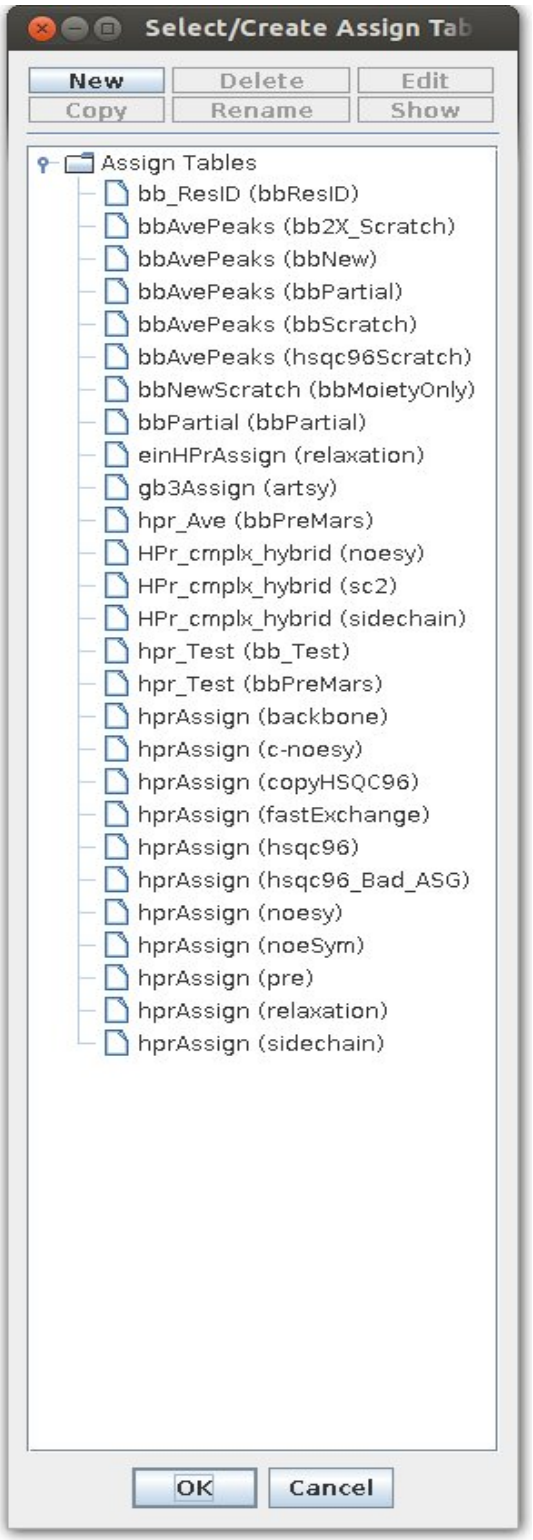
To create multi-chain sequences enter the longest sequence first then pad with G or A up to nearest multiple of 100. For the complex EIN (1 → 259) with HPr (301-> 386) I used:

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.

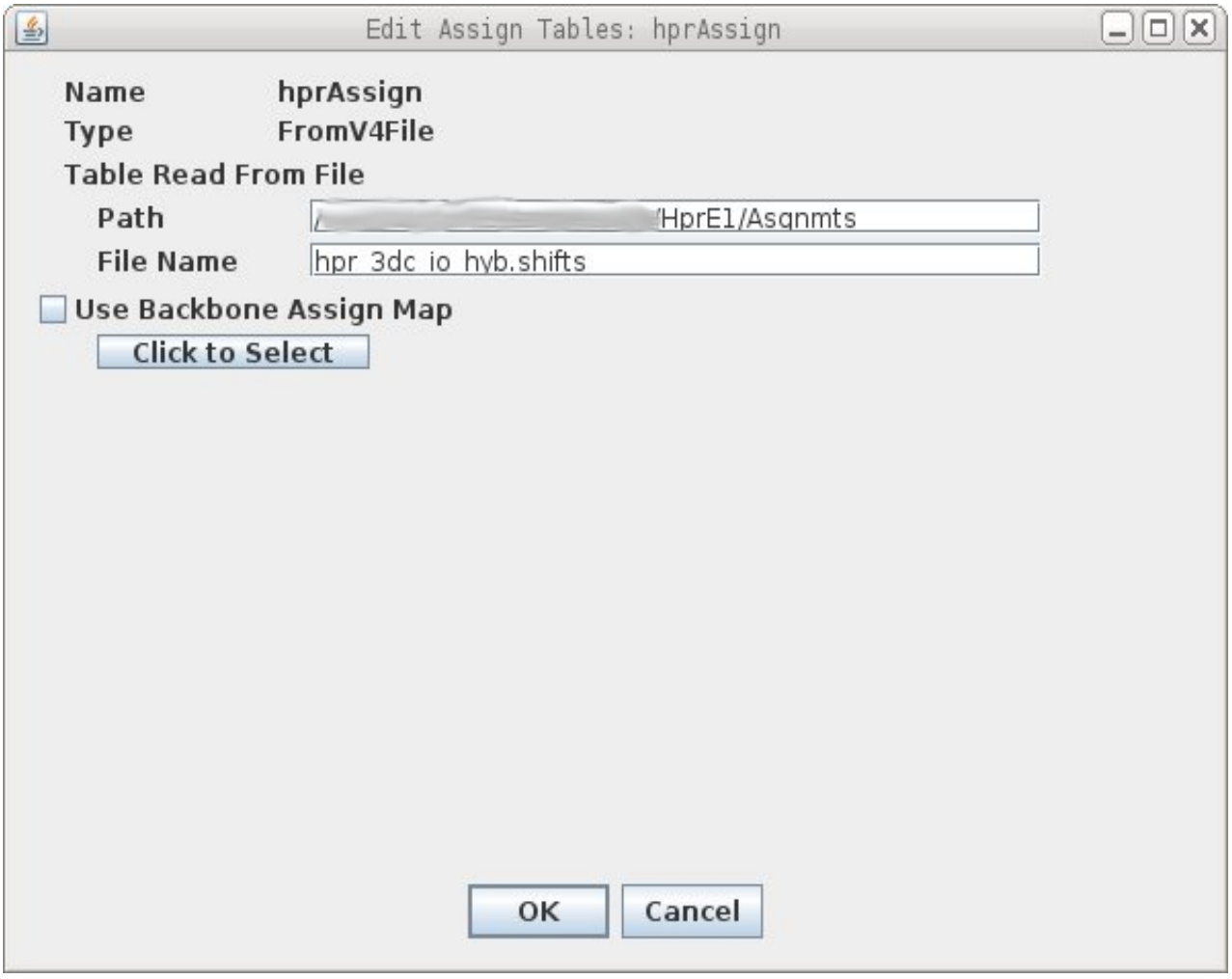
Currently there are 3 types of Assign Tables:

- 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
  - Merges list of assign tables to form 1 table. Assigns from first table take precedence over assigns from tables lower in list.

Edit 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.



Must enter directory of file, ie Path, ad File Name.

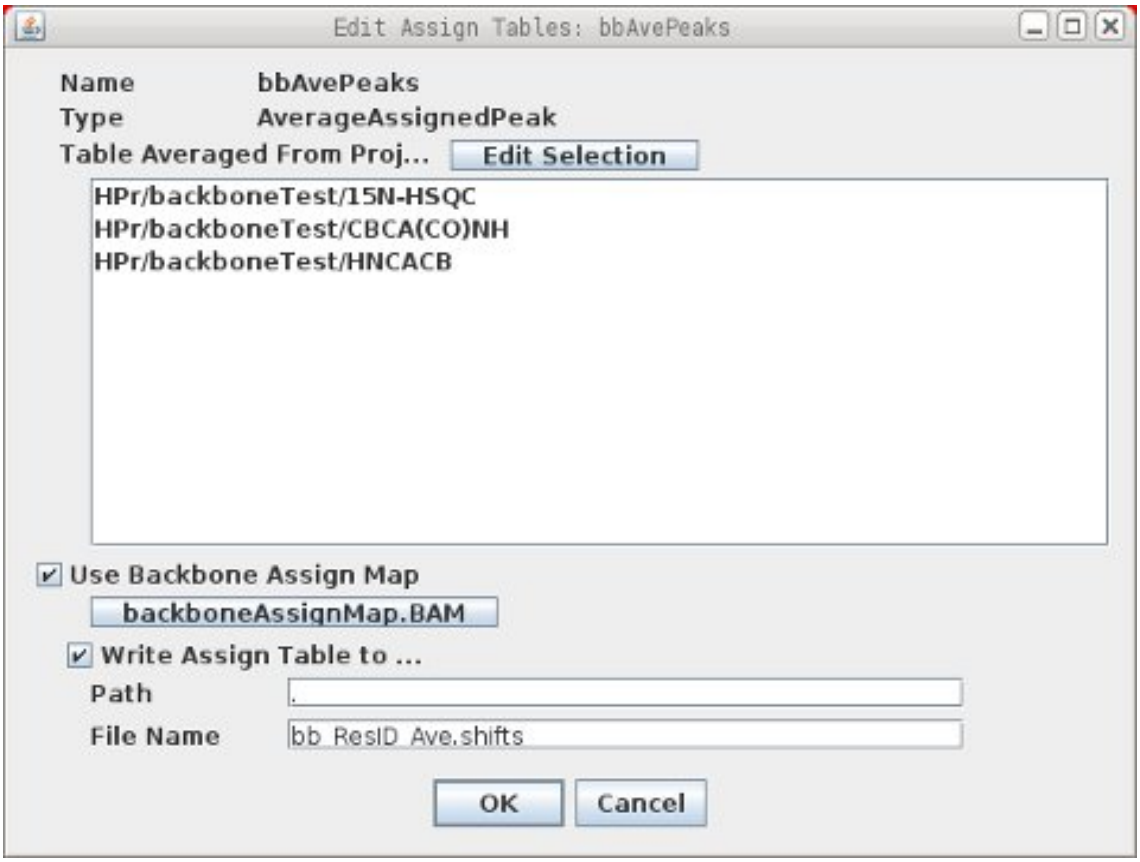
The format of the .shifts file must be in the PIPP V4 format.

The Backbone Assign Map should only be used with Backbone Assign Study. For all other studies this should not be set.

Edit 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.



This example defines the assignment table as the average of the assigned peak-picks from the HSQC, CBCA(CO)NH and HNCACB.

By default the list is empty and you must click Edit Selection to bring up a dialog that lets you select which experiments to use in the average. As you collect more experiments you must re-edit this list in order to have the peak-picks from those experiments be included in the average.

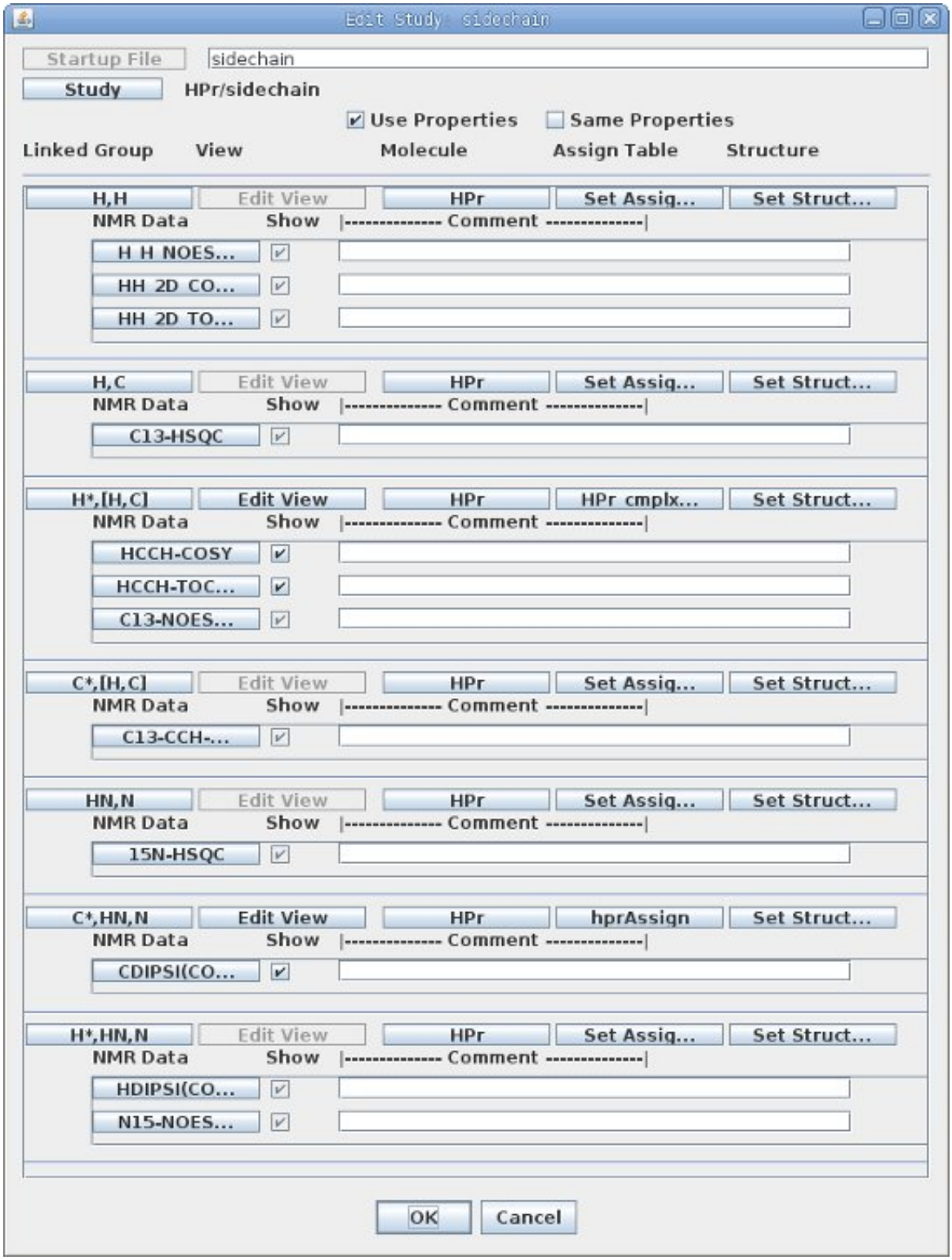
The Backbone Assign Map should only be used with Backbone Assign Study. For all other studies this should not be set.

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 assign study. The AverageAssignedPeak never reads in this *.shifts file.

Edit Study: Sidechain Assign Dialog

This dialog can be obtained in two ways:

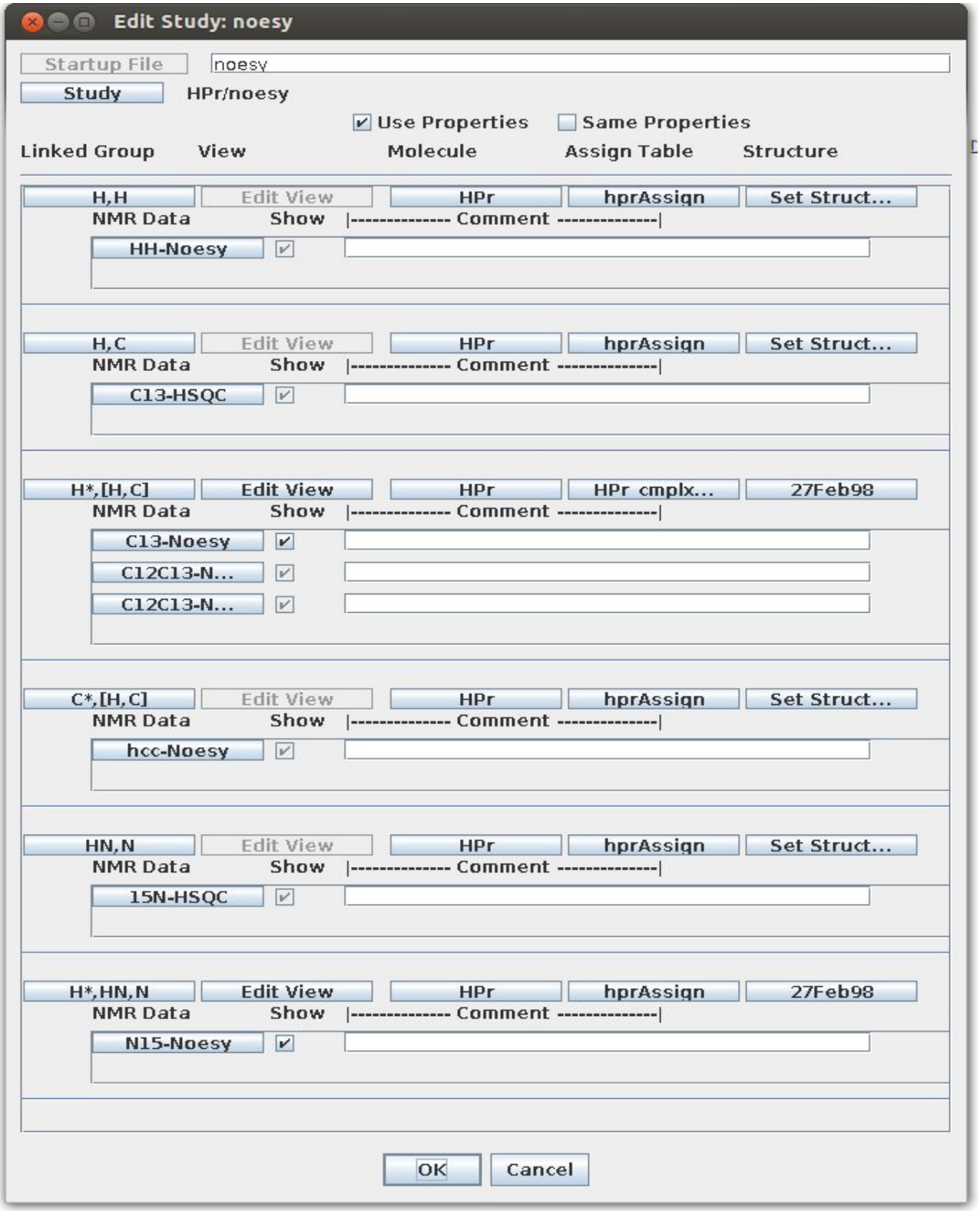
1. Creating new study from New Study Dialog Panel with Sidechain Assign Study selected.
2. By clicking on the Edit button on the XippPanel when a sidechain study is selected.



Edit Study: Noesy Assign 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.



Edit Study: Sidechain Assign Dialog
Edit Study: Noesy Assign Dialog

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

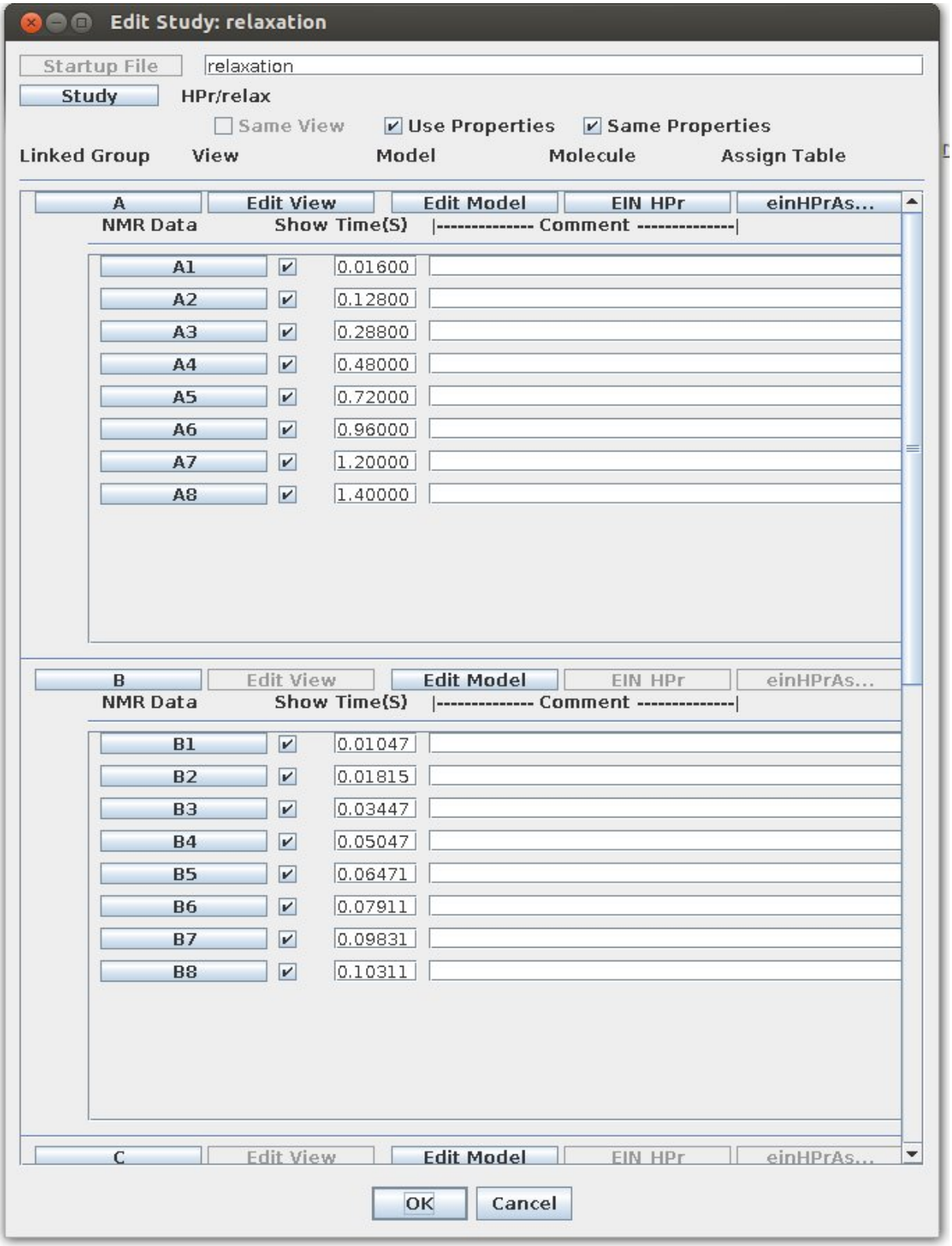
Refer to the page 'Edit Study: Backbone Assign Dialog' for a description of the buttons.

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 sidechain.xipp and noesy.xipp in these examples.

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.



Edit Study: Relaxation (T1, T2) Dialog

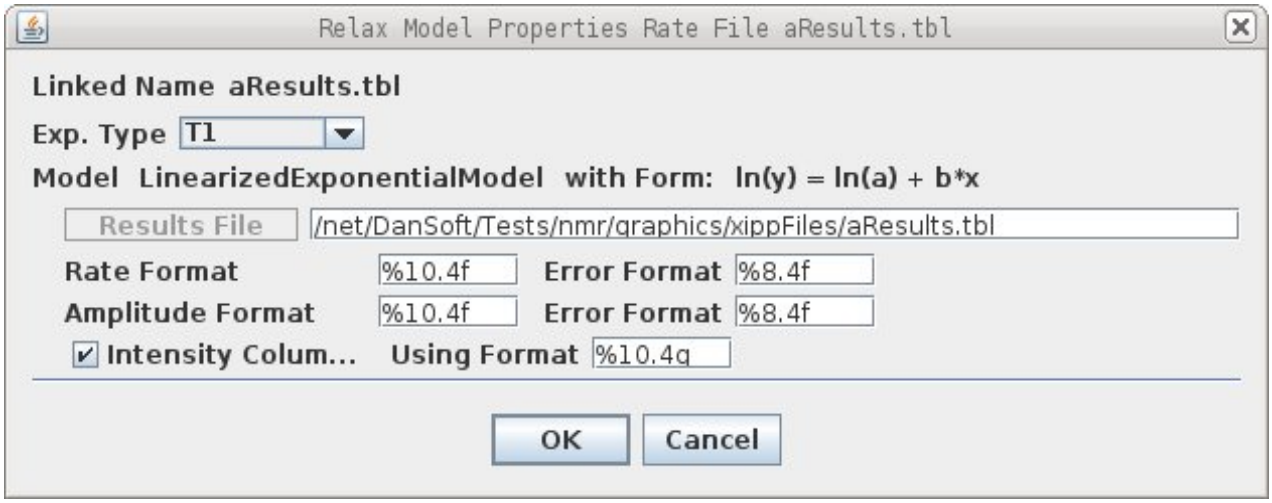
This dialog defines 2 sets of T1 and T2 (or T1rho) with 8 NMR experiments each. In order to increase the number of NMR experiments or increase the number of sets of T1 or T2 groups you need to edit the Python file configTree.py which by default is installed at ~/Xipp/v1/lib/nmr The part that needs to 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:



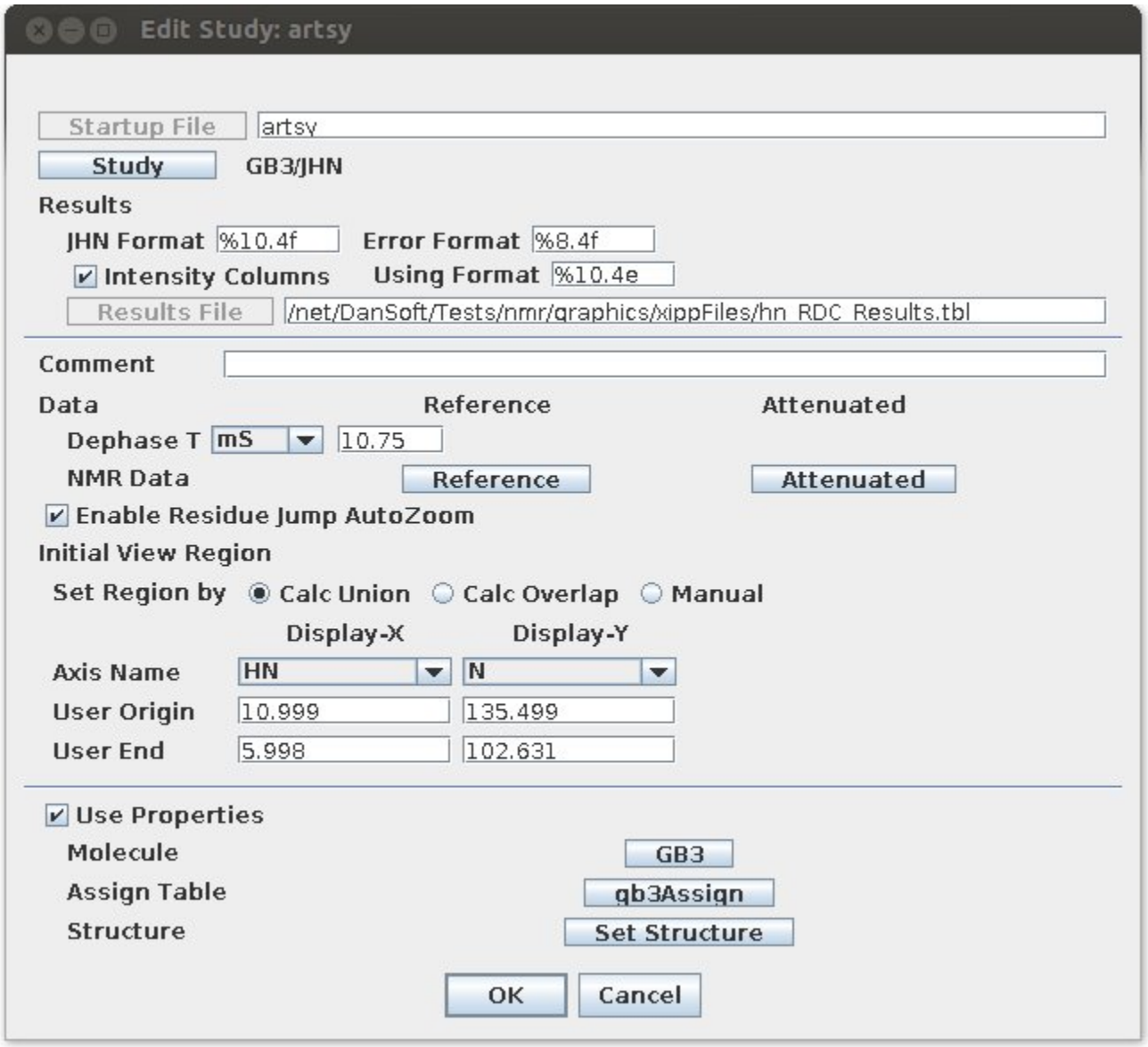
Changing Exp. Type only changes a label in the output. The Exp. Type is not important for fitting the data to the LinearizedExponentialModel.

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.

J_{HN} RDC ARTSY Study Panel

This dialog can be obtained in two ways:

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



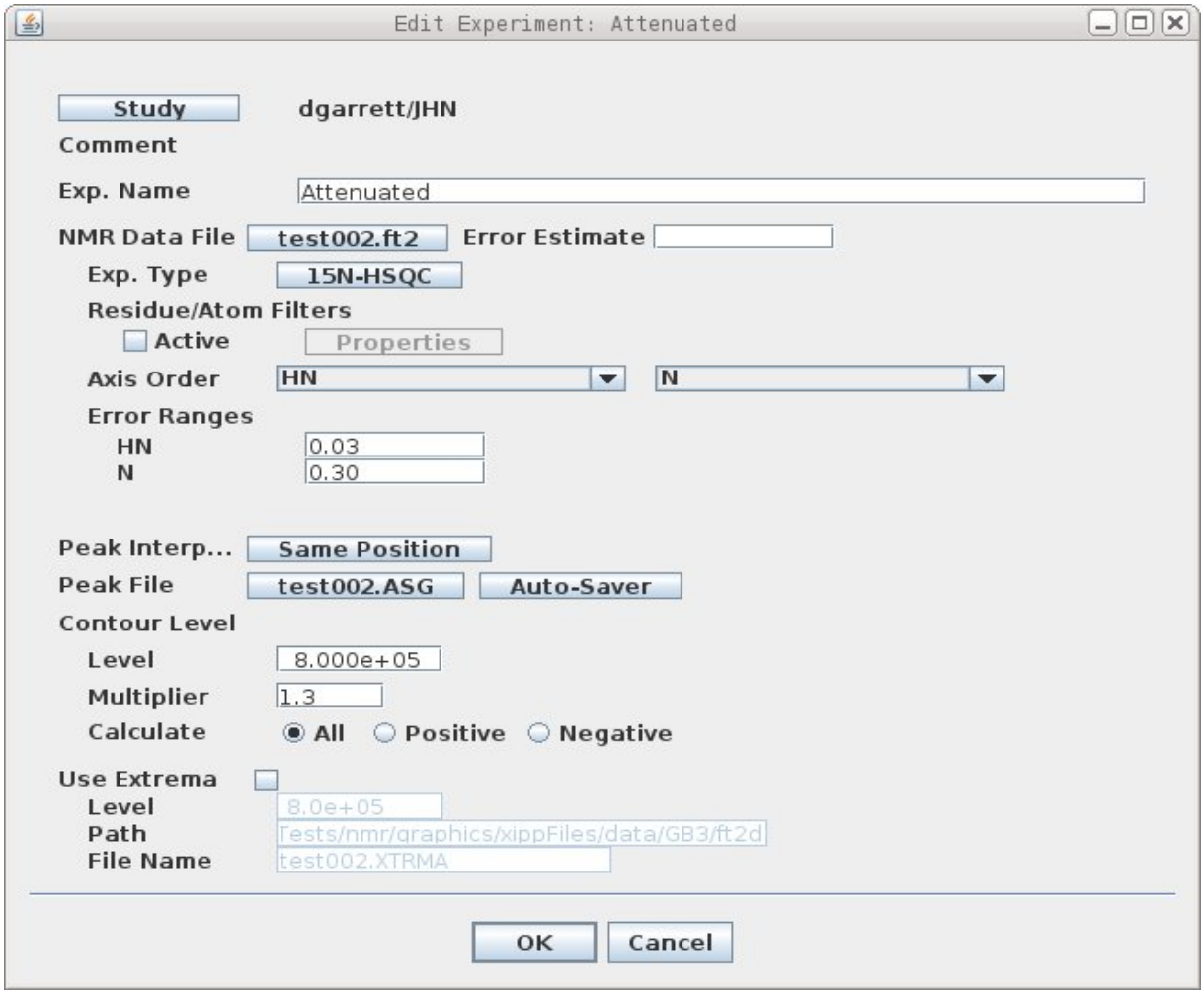
Edit Study: J_{HN} RDC ARTSY Dialog

This dialog defines 1 ARTSY Study:

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. 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.

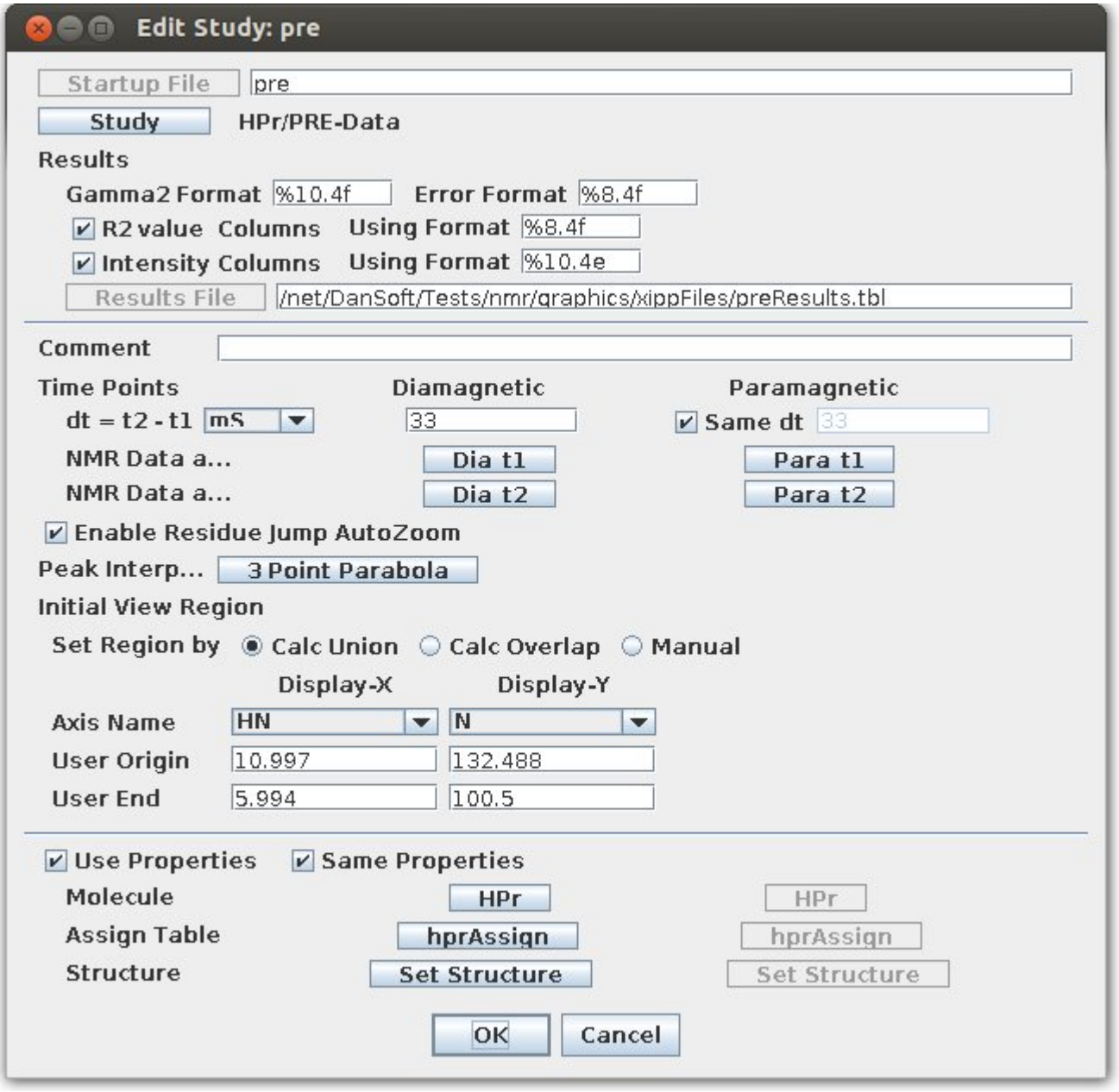


Clicking OK at the bottom of the Edit Study Dialog will save all of the properties into the file based on the study name, ie artsy.xipp in this example.

Edit Study: PRE Study Dialog

This dialog can be obtained in two ways:

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

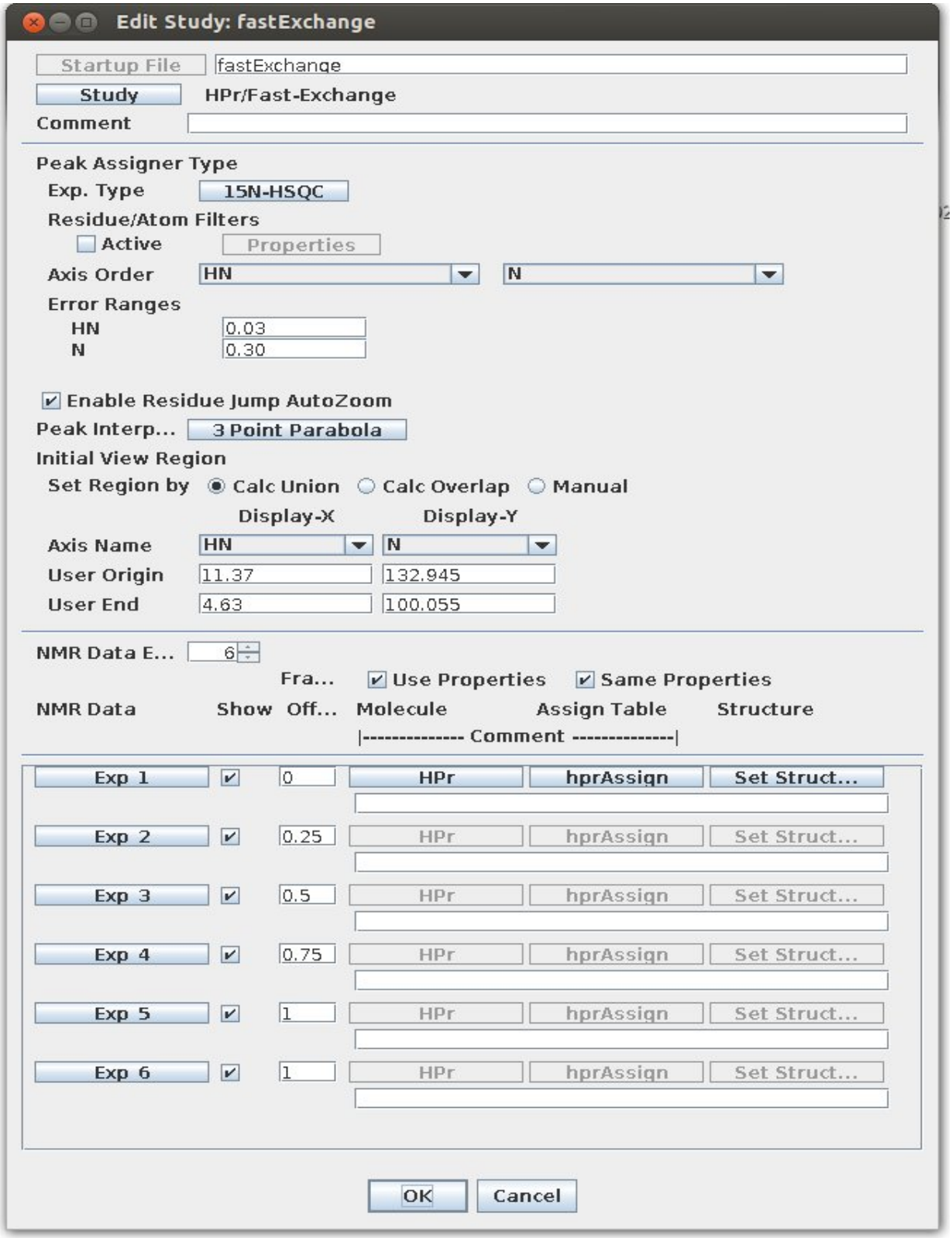


The PRE Study Dialog is very similar to the ARTSY Dialog except that 4 NMR experiments are used to define the two-point PRE.

Edit Study: Fast Exchange Dialog

This dialog can be obtained in two ways:

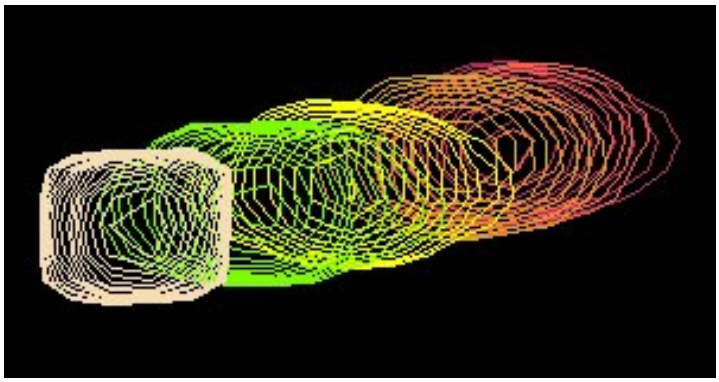
1. Creating new study from New Study Dialog Panel with Fast Exchange Study selected.
2. By clicking on the Edit button on the XippPanel when a Fast Exchange study is selected.



Edit Study: Fast Exchange Dialog

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 in 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.