Version	Date	Changes
1.21.7	07/21/21	Added ability to output Peak-Pick data in PCK format in units Hz and Points via Auto-Saver button from NMR Data Experiment Dialog. See createSetStudies.pdf (pages 8, 10, 14 & 15) for details. Fixed Mars Perl scripts that failed to run on Linux due to Perl deprecating $[= 1; comand which set base for arrays to 1 in scripts runmars and runmars_noIter. Since $[was deprecated all arrays in the Mars scripts had their base set to 0 instead of 1 which required checking every line for an array to ensure its base was 0 instead of 1. Multiple minor bug fixes.
1.18.10	10/25/18	Added PPM offsets to NMR Data Experiment for each observed axis. The value is added to the observed Peak-Pick position prior to comparing to assignment table. The PPM value for a Peak-Pick in the peak-pick file does NOT get changed by this value, but Shifts created from a Peak-Pick are offset. Moved Button labeled 'Reference' from NMRPipe File Chooser dialog to NMR Data Experiment dialog so that the reference information can be shown more easily when selecting Axis Order. Created properly bonded AmbiguousAtoms for non-stereo assigned Methyl groups: Leu {CD1|CD2, HD1#|HD2#, CD2|CD1, HD2#|HD1#} and Val {CG1|CG2, HG1#|HG2#, CG2|CG1, HG2#|HG1#} with bonding defined so that CD1|CD2 is bonded to HD1#|HD2# and CD2|CD1 is bonded to CD2#|CD1#. This is the same way that PIPP did it, but I had not gotten around to including this in Xipp. This is really useful for analysing HCCH COSY/TOCSY data. Added some backbone experiments to Sidechain Study panel so that the assignment table in the Sidechain Study can be defined as an average of assigned peaks using the same (or copied) peak-pick files from the Backbone Study. Added menu item to Symmetry menu to allow Peak-Picking of the selected Symmetry Peak. This is in the Menu from the TableWindow S+ button next to list of Symmetry Peaks and is the Menu Item labeled 'PeakPick Symm.' that is just above the Copy Table menu option. This makes it easier to create sidechain assignments when the symmetry peak is for a Carbon that has not yet been assigned, ie can't easily jump to it since it is not in assignment table. After Peak-Picking the symmetry peak and selecting an assignment you can then jump to the 13C plane for the carbon atom since it is in the assignment table. Added menu item labeled 'Auto Assign Peaks' to Experiment display buttons just above 'Contour Levels' menu item Canvas Window to disable automatically selecting an assignment when a peak is picked and the assigner rules only show a single assignment. I am worried that the label 'Auto Assign Peaks' may be mis-leading and confused with fully automated assignment. This is useful when you are trying to determine offsets from data between different samples (ie fully per-deuterated and fully protonated). If the assignments are an average of all assigned peaks then the deviation shown in the table is calculated after the new peak is assigned if it is automatically assigned which is the default when there is just one possible assignment found. Turning this off prevents the peak from being automatically assigned so the offset from the assignment table to this experiment can be determined. Added ability to manually create a backup Jar file on demand. A backup Jar file was previously only created when Xipp started and finished. The Canvas Window File menu option 'Save-Data' will after saving all of the data now create a Jar file with the file name in the format <studyName>_M_<dateTime>.jar In addition the xippOutput.log file will record whenever a Jar file is created. One problem not resolved is that the xippOutput.log file contains all the output from all shown Studies. When the Jar file is created a copy of the xippOutput.log is put in the Jar file which will contain output from other Studies.
1.17.11	11/07/17	Added new Studies to assign series data such as T1, CPMG, PRE, Dispersion, and Delta-Rate. It plots the data on the screen as it is picked and writes out a table for easier analysis with relaxation software. Sorry no hard-copy plots.

Set property labels to red in dialog panels to indicate which properties need to be set or have been set incorrectly.

Fixed display of arbitrary labels over peak-picks in canvas window.

Minor bug fixes.

1.14.10 10/22/14 Created XippPanel GUI to create, edit and manage studies, experiments and properties. The XippPanel is shown when xipp starts with no arguments.

Created examples and Studies for: Single Experiment, Backbone Assign, Sidechain Assign, Noesy Assign, Relaxation (T1,T1), JHN RDC ARTSY, PRE (2 time point) and Fast Exchange.

Replaced using Python file *.py (ie data.py and graphics.py) as property files with a single XML file for each study. Each XML file is a *.xipp file which defines all of the properties for a single study. This was needed because there was a size limitation with the *.py files. Each entry in the XippPanel is a separate *.xipp study file.

Added Vector Peak Picking which is useful for a Fast-Exchange study in which a peak for a single residue moves position due to changing concentration of an unlabeled ligand in different spectra. The two ends of the vector are defined by the user by doing the mouse down at one end of peaks and releasing the mouse at the opposite end of the peaks.

Added support to start CAPP, ps_contour and MARS from within Xipp. All three are external C programs started from within Xipp with results read back into Xipp, (except for ps_contour which crates a post-script plot).

For triple resonance Exps order of atoms in NMR data is determined by spectrometer frequency of each axis and gyromagnetic ratio of atom type (H, C, N).