Data manipulations with VNMRJ 2.3 A

Version 2.3 A of VNMRJ is currently installed on **v700, i600** and expected to be on **u500** before the end of February. The rest of the spectrometers and data stations will follow soon after u500.

The main difference to the older version of VNMRJ is the data manipulation and directory navigation. This help file shows the new way of managing NMR data.
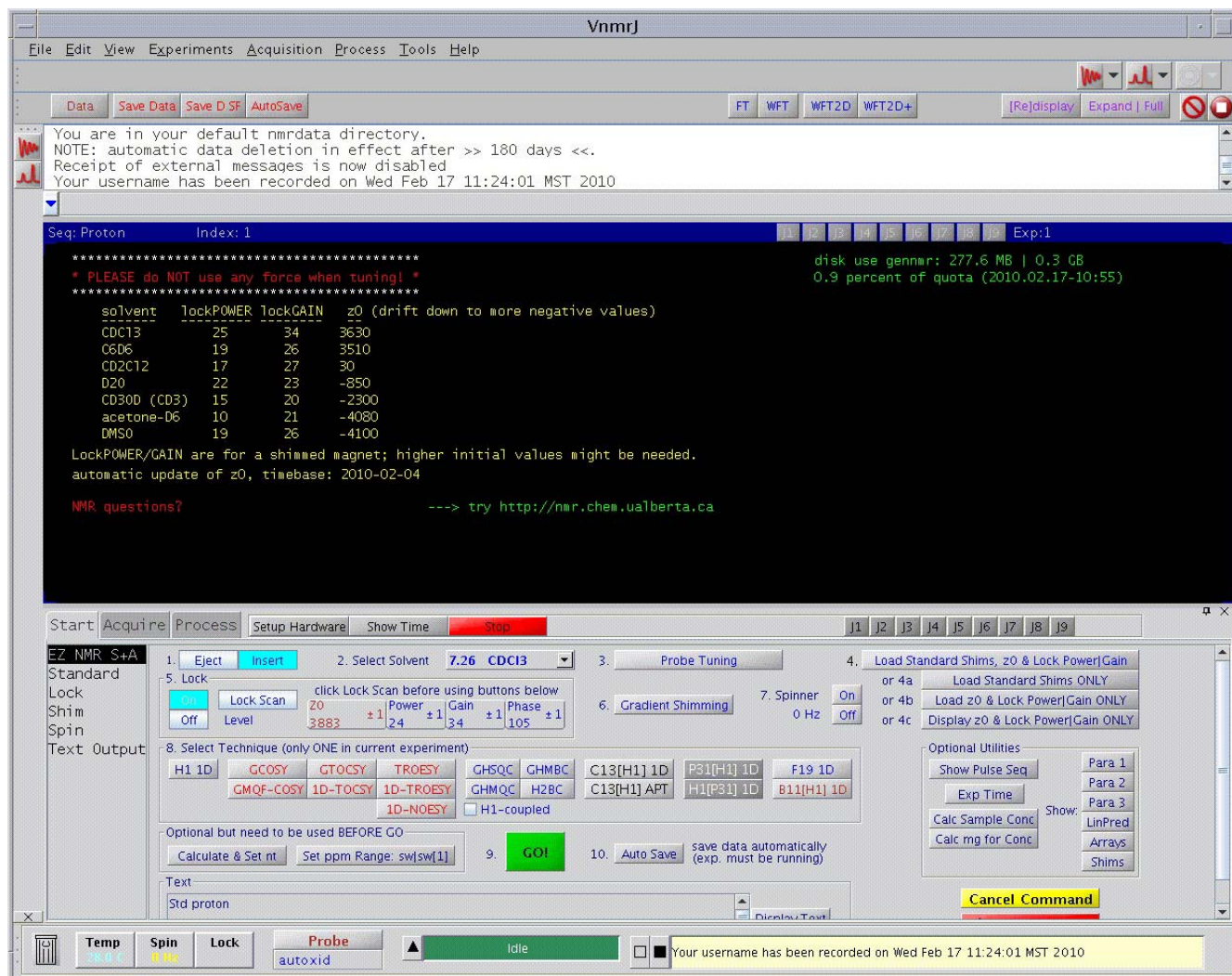
The VNMRJ 2.3 A interface is shown in Figure 1.

Figure 1: VNMRJ 2.3 A interface

There are fewer data handling buttons now in the top left corner (Figure 2). Only saving of data in free format or standard format (SF) plus AutoSave are available. The rest appears in a separate window which can be accessed by a single click on the **Data** button. The new Data Manager window (Figure 3) is used to navigate the directories and to perform all data-related operations such as saving, loading, renaming data etc. It opens in the **default data directory** (also accessible at any time by clicking on the **Data Dir** button). As indicated by the red text at the bottom, desired files or directories should be highlighted with the left mouse button and entered with a middle mouse button click onto the desired line.
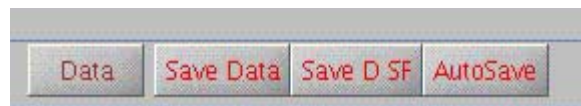

Figure 2: data manipulation buttons

Navigation to the HALL directory is used in the following example (Figures 4 to 6).

Figure 3: Data Manager window

Note that the Current Working Directory is always visible just above the list of directories.

Instead of using the mouse to obtain the directory name, it can also be typed right on the Directory Navigation line by appending HALL to the existing directory information.

Important when typing: **files and directories are case sensitive**. Special characters as well as empty space are replaced automatically by _.
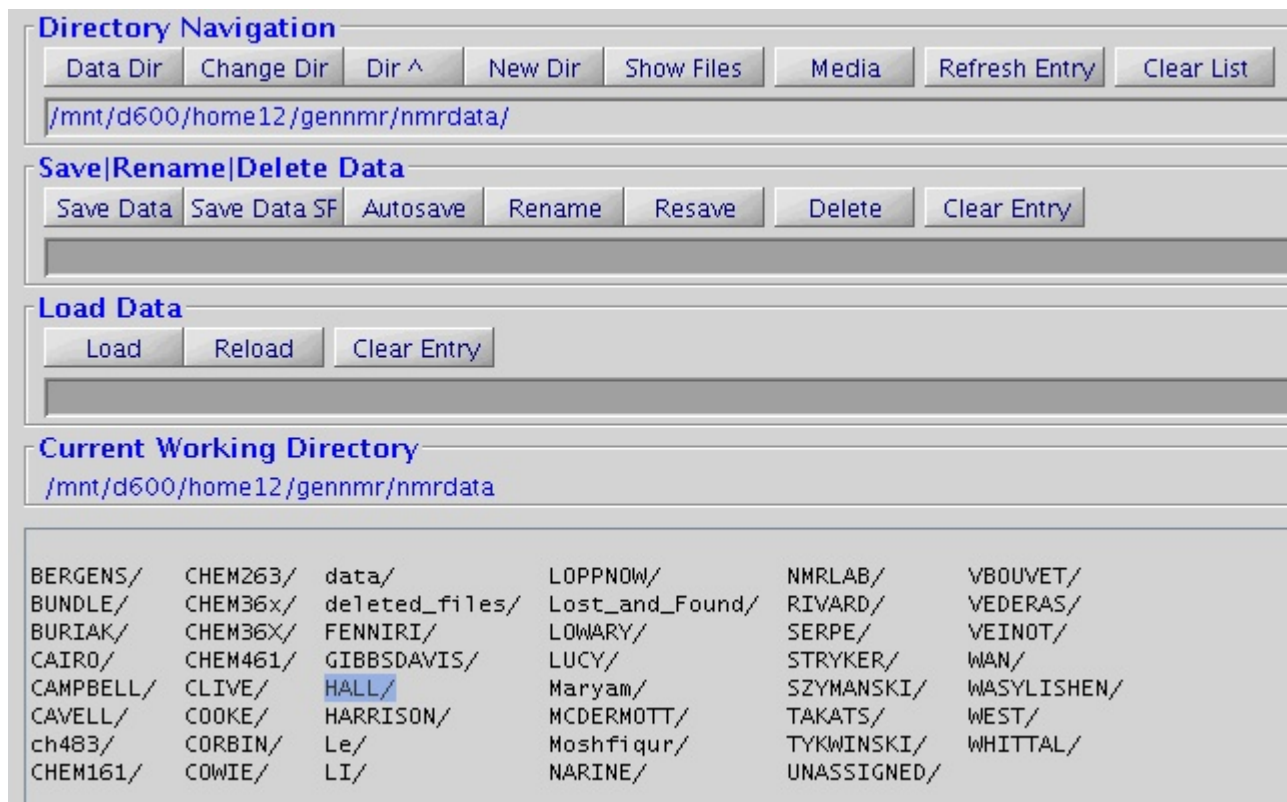
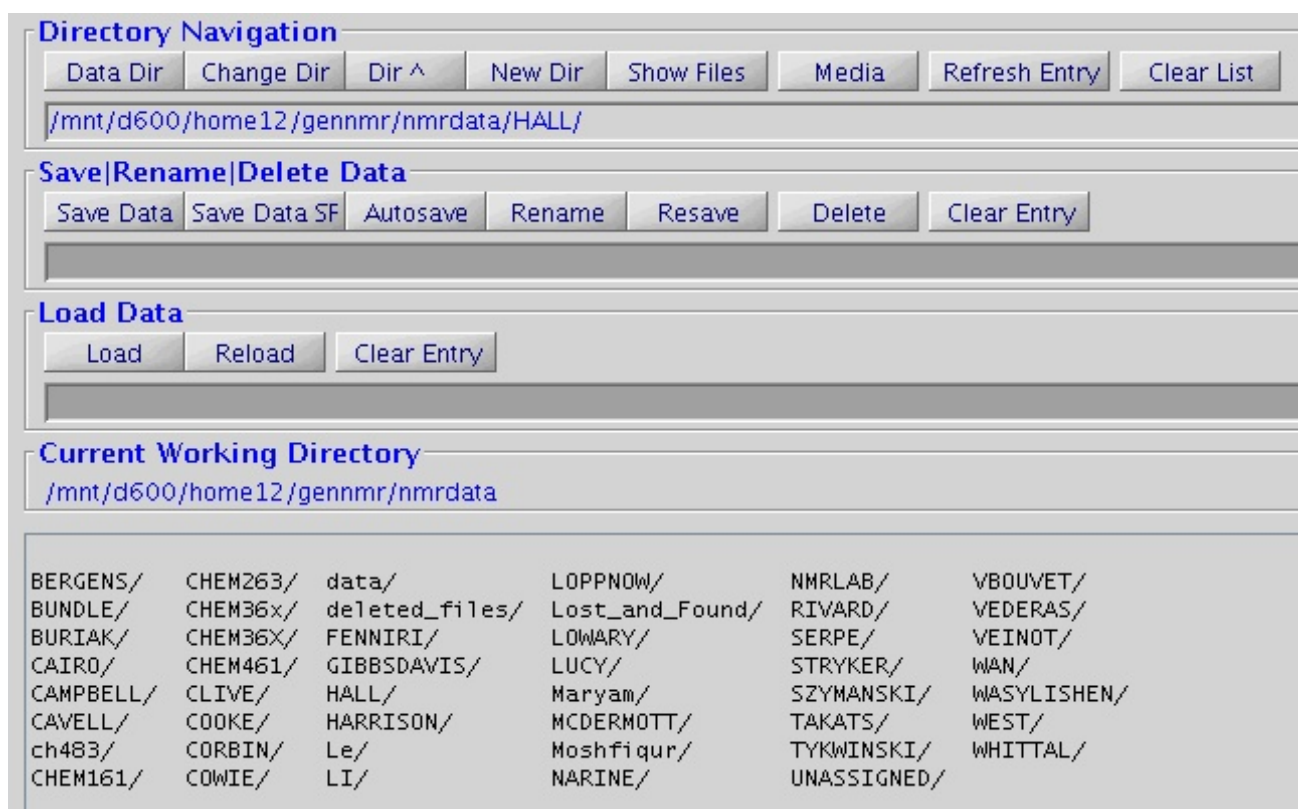Figure 4: Desired directory highlighted with left mouse button

Figure 5: Desired directory entered on the Directory Navigation line by typing or mouse middle click
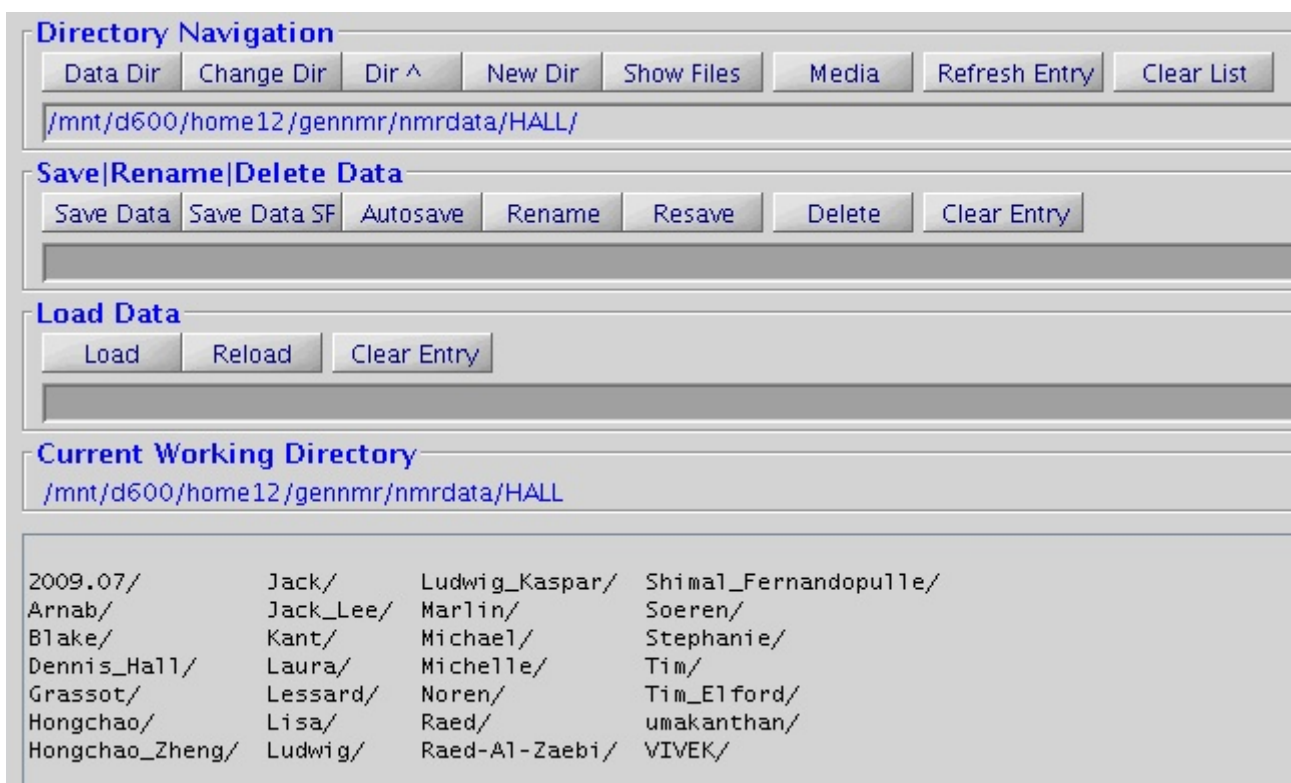
Figure 6: Directory content appears after clicking on the **Change Dir** button

The procedure has to be repeated until the desired directory is reached.

In this example it is Noren and 2010/01/. The desired file (*) is highlighted in Figure 7 then put on the Load Data line in Figure 8 with a click on the middle mouse button.
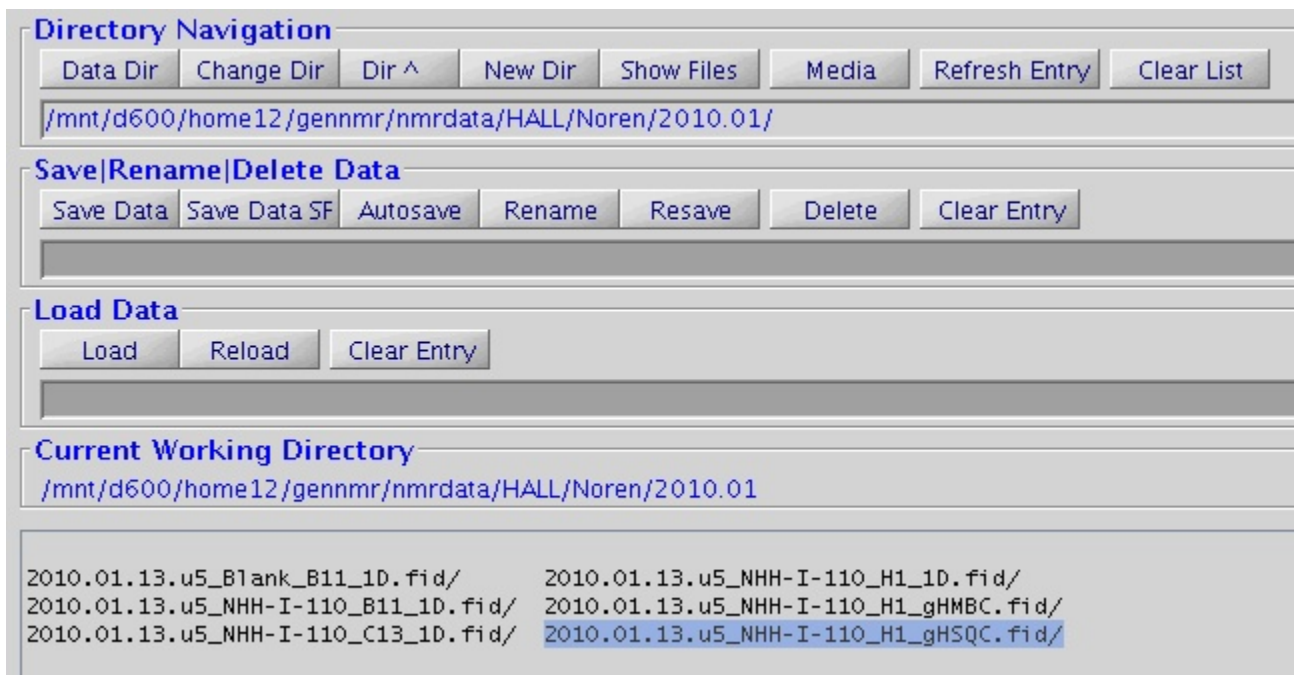

Figure 7: Desired directory after more Change Dir; the fid of interest is highlighted
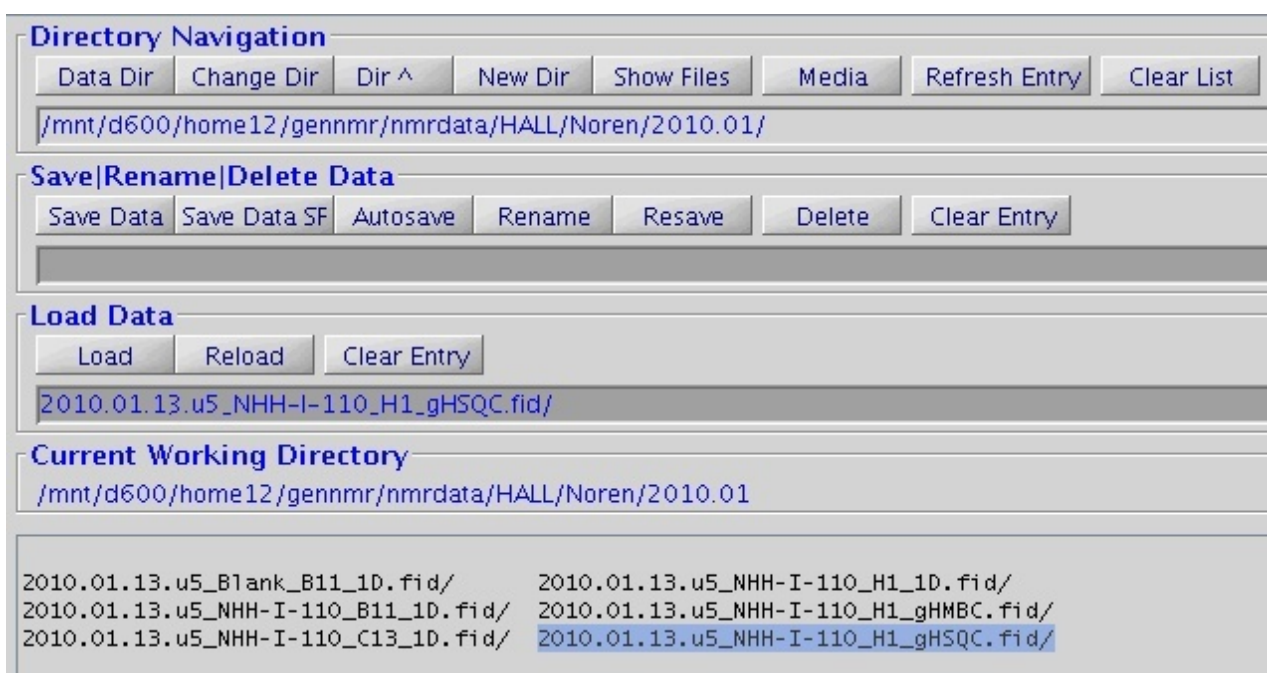
Figure 8: Desired fid on the Load Data line

A click on the **Load** button completes the procedure and the data 2010.01.13.u5…...gHSQC.fid get loaded and are ready for processing.

Saving the data requires simply typing of the desired name on the Save|Rename|Delete Data line followed by a click on one of the Save buttons.

Save Data	free-style naming but **files and directories are case sensitive** and special characters as well as empty space are replaced automatically by _
Save Data SF	a format like the one shown in Figure 8 is chosen with the user-selectable text in the middle of date/spectrometer and nucleus/technique information
Autosave	spectrometer saves data automatically in standard format; AutoSave now requires confirmation by the user in a separate pop-up window.
Rename	allows renaming of selected data
Resave	saves the current file with new parameters (e.g. after re-phasing, changing the text etc. – the fid itself is unchanged); in essence only procpar inside name.fid is updated
Delete	deletes data without an undo or undelete option
Clear Entry	clears the input line

The procedure is not complicated – it just needs a little bit of trying to get the feel for it!

(*)   VNMRJ stores data always in a directory containing the actual FID, procpar, text etc. The directory name always ends in .fid.