Parameter File Handling In TopSpin 3.0

Parameter Files = pulse / cpd / Au / python programs, macros, shape/gradient files, parameter sets (such as PROTON, ...

1. **Parameter files can be located *in arbitrary directories* in the file system. See below how to set up such directories and make them known to TopSpin.**
2. Bruker parameter files are available *after expinstall* in TOPSPINHOME/exp/stan/nmr in their standard subdirectories, e.g. subdir=lists/pp for pulse programs.
3. In order to setup additional directories containing parameter files, proceed as follows:
   - Make sure *expinstall* has been done
   - Type edpul or edcpd or edmac or edpy, ...
   - Select *Manage Source Directories* from the *Options* menu
   - A dialog comes up containing the Bruker standard directories. Add your own directory, one per line, by entering them using the keyboard, or the Browse button. When using the Browse button, navigate the file explorer to the desired directory, mark the directory in the address field, type CTRL/C to copy it, move the cursor back to TopSpin, type CTRL/V to paste it into the desired parameter field. Click OK when done.
   - The result is stored in the file *<your topspin properties directory>/parfiles-dirs.prop* and is therefore user-specific: Every system user may set up an own directory list. In principle, you could generate this file manually yourself using a text editor or a script, but beware of typing and format errors!
   - TopSpin must be restarted before changes become effective. The reason is that setup is possible while background processes such as acquisition or automation are running, and changing the directory list might affect the parameter files used. When starting TopSpin, the user's *parfiles-dirs.prop* file is copies to *TOPSPINHOME/conf/parfiles-dirs.prop* which is the file actually used at runtime.
   - The next section shows that the order of the directories plays an important role!
4. Parameter files are used by a number of TopSpin commands. The command *zg* evaluates the parameter PULPROG. Assume PULPROG=*cosyph*. If no special directory list has been generated by the user, *cosyph* will be found in Bruker's standard directory, and will be used for data acquisition. However, if additional directories have been set up, several pulse programs with name *cosyph* could be present. *zg* will take the first one found by scanning the pulse program directories list top down. You may for example give Bruker's pulse programs highest or lowest priority, or even remove the Bruker standard directories from the list!
5. When typing *edpul, edcpd, edmac, edpy, edshape, edgp, rpar etc.* a window comes up containing the respective items. The contents of the window is displayed from data bases in xml format, built from the parameter directories. The data base allows for effective searching and sorting. It also takes care that directory contents and data base are always consistent, even if parameter files get modified outside TopSpin with some text editor. The data base is only used for the display commands *edpul* etc., while acquisition and processing commands get the files directly from the directory where they are stored.
6. TopSpin does not support changing files in the Bruker standard directories. For example, it is not allowed to change a pulse program stored in *TOPSPINHOME/exp/stan/nmr/lists/pp,* nor is it permitted to save own pulse programs there. For this reason, Bruker provides a subdirectory *TOPSPINHOME/exp/stan/nmr/lists/pp/user* where user-defined pulse programs can be stored and edited. Of course, you may store your pulse programs anywhere as outline before, but this subdirectory is available by default. Such *user* subdirectories are also available in the other standard directories, e.g *TOPSPINHOME/exp/stan/nmr/lists/cpd/user*.

7. ***File --> Export...*** opens a browser dialog and exports (= copies) the selected items in the *edpul, edcpd, ..., rpar/wpar* window to the destination directory selected in the browser dialog.
8. ***File --> Import...*** opens a browser dialog and imports (= copies) the items selected in the browser dialog to the directory currently selected in the *edpul, edcpd, ..., rpar/wpar* window, and updates the window.
9. In the *rpar/wpar* window, the ***File*** menu contains a menu item *Files*. It show the contents of the selected parameter set (e.g. the files *acqu, proc, ...*) and allows one to view their file contents.
10. Pulse/AU/CPD/... programs and parameter sets can be classified by adding respective tags to the pulse (or) program.
    The following tags are available: (here displayed in form of examples)
    $CLASS=selective
    $DIM=2
    $TYPE=mytype1
    $SUBTYPE=subtype2

    The following is also possible: (and item belonging to several categories).
    $CLASS=selective, selective2,
    $DIM=2
    $TYPE=mytype1
    $SUBTYPE=subtype2, subtype7,
    (Note: The last item of MUST end with a comma in these cases!)

    WARNING: The tags must be preceded by the *comment indicator* of the respective program type, e.g. ";" for pulse programs.

    Parameter sets can be classified as follows:
    Add a new file called "comment.txt" in the parameter set's directory (where the *acqu* and *proc* files are located.

    This file must be a text file. Here is a sample contents:
    $CLASS=selective
    $DIM=2
    $TYPE=mytype1
    $SUBTYPE=subtype2

    Other tags:
    $COMMENT=2D HSQC with refocussing of C chemical shift
    $RECOMMEND=y
    Only items containing this tag will be shown on the list display when the check button "show recommend items only" is enabled.

11. Changing tags such as $COMMENT=
    When you add or change tags pulse programs, parameter sets etc. you must perform as follows so as to enable TopSpin to dissplay the changes when typing *edpul, rpar*, etc.
    - exit topspin
    - cd <topspin home>*/prog/curdir/*<user>/db/Local
    - delete the entire contents of this dir
    - restart topspin