

## VNMRJ Customization

VNMRJ while is a user friendly interface, it can also be difficult to use when one tries to set up a non-Varian supplied sequence or outside the packs like BioPack, ChemPack, or solidspack. The reason being is that the various panels below the graphics are that allow control of the experiment acquisition, processing, and display may not be relevant for the new sequence under use. The standard use of the VNMRJ software requires the user to copy a file from `/vnmr/templates/layout/xxx`, where `xxx` is a directory for a pulse sequence that is closely related to the current one to the local directory `vnmr/sys/templates/layout/yyy`. The `yyy` is the name of the pulse sequence. When a pulse sequence is loaded the the parameter `seqfil` is consulted to load the appropriate panels from a file `yyy` either in the local templates or the `/vnmr` directory.

For example, if one modified `gNhsqc` to `gNhsqc_v2` then when `seqfil='gNhsqc_v2'` the panel pages will all be similar to a 1D experiment. One way is to do a copy as follows (assuming `biopack` is installed in `/vnmr`):

```
cp -r /vnmr/templates/layout/gNhsqc ~/vnmr/sys/templates/layout/gNhsqc_v2
```

Thus, for every new version a new file needs to be copied.

However, the standard VNMRJ has been modified to avoid this step. The new default would automatically set a 1D, 2D, or 3D acquisition, process, display, and plot panels that resemble BioPack depending on the type of experiment. The files that are modified to enable these are in the directory `/vnmr/templates/layout/default`.

*2Dplot.xml, 2D.xml, 3DParameters.xml, 3Dplanes.xml, acq.xml, disp.xml, F1F3plot.xml, F1F3.xml, F2F3plot.xml, F2F3.xml, plot.xml, Process2dint1.xml, Process2dint2.xml, Process3dint1.xml, Process3dint2.xml, Process3dint3.xml, Process.xml and proc.xml.* There are two new files *Acquisition2DA.xml*, and *lek.xml* (these files are called by `acq.xml`). The files `acq.xml`, `proc.xml`, `disp.xml`, and `plot.xml` call the other files in setting the environment. There is a directory called **customization** in `/home/vnmr1` of `unity500D`, `inova500D`, and `inova600D`, and there are two files **custom\_default.tar** and a macro **lek**. Place the tar file in `/vnmr/templates/layout/default` and expanded to get these files. It is encouraged to backup the originals before doing so. Copy the macro **lek** to `/vnmr/maclib`.

These are simple text files and one can inspect them to see the changes. For the implementation to work, BioPack should have been installed in `/vnmr` as `vnmr1` (see `BioPack_Install` manual). Before any future BioPack complete install is implemented one should backup the above files and recopy them so that the customization is preserved. There is good chance that these might become standard in future BioPack releases. However, the `lek.xml` related changes are custom for this site.

The `Acquisition2DA.xml` is invoked by `acq.xml` if the parameter `ni` exists, characterizing a 2D experiment and the panel changes accordingly. If you are invoking a 3D parameter set the Acquisition page will change to a 3D panel as `ni2` also exists in addition to `ni`.

An option to show almost all parameters in a Pulse Sequence page for a pulse sequence from Lewis Kay pulse sequence library is also implemented. The *lek.xml* is invoked by *acq.xml* if the parameter *lek* exists and set as *lek='y'*. Then a Pulse Sequence page will appear that has Lewis Kay pulse sequence parameters. Since this *lek* parameter doesn't exist by default, after the user loads a Lewis Kay experiment parameter set, call the macro ***lek*** (macro resides in */vnmr/maclib*) then the page will be present.

These modifications are implemented in *inova600D*, *inova500D*, and *unity500D*. If you don't like them they can be reset to default settings by renaming the *.orig* files.