NMR Felix 95.0: A Beginner's Guide

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To begin to use Felix 95.0, you first need to type at the terminal prompt

#source /zhadum/biosym/cshrc

You can then start felix using

#FelixX

The terminal from which you open Felix will now note all of Felix's activities. Any requested functions, error messages, or requested numerical values will be printed here. As the program starts up it will ask whether you want to open a database file "file.dba." For the first time, click on "yes." (This file is important if you want to retrieve your worked up data from a previous session.)

When you start up Felix, the main window will pop up with a **menu bar** on the top. The bold-underline type will be used here to specify when you need to click on a button from this menu, and simple underline when you need to click on a prompt button.

Importing and converting data to Felix readable format:

1. Create a directory labeled *felix230/fid* in your home directory if it doesn't already exist. At a Unix prompt, enter:
   cd
   mkdir felix230/fid

2. Move the spectrum directory (*name.fid*) to this new folder, e.g. for a spectrum *datedata/name.fid*:
   cd
   cd *datedata*
   cp -r *name.fid* ~/felix230/.

   or better (I've [cgf] had less trouble with tar than with cp):
   cd
   cd *datedata*
   tar -cvf *name.fid nametar*
   cd ~/felix230
   tar -xvf ~/*datedata/nametar*

3. Check to make sure you have a folder felix230/data in your home directory. Create one if absent:
   cd ~/felix230
   dir
   if *data* not present, then:
   mkdir data

4. Under **File** find the option for import data, and choose the type of data (Varian, Bruker, etc.) you would like to import.

5. An import window will pop up requesting information on the path and names of input and output files:

Input file:	*name*.fid
Data Prefix:	/*homedirectory*/felix230/fid/
Output file:	*name*.dat
Data prefix:	/*homedirectory*/felix230/data/

If all went well you should have a data matrix folder with **.dat** prefix in your data folder.

Data Processing (1D and 2D)

1. For LB, switch to **1D mode**, and then under **File** Read data.
2. From **Process** select Windows:view, click on time domain, and then OK at the confirmation. You will be prompted for a source through a data source window. Select a function (e.g. exponential function). Click on work. At this point a window with a fid and the function will appear. Adjust the multiplier function using the black dial and cursor on the left side.
3. Keep this from the window displaying the fid.

1D Spectrum

- For a 1D fid, from the **User** menu select E-Z 1D transform.
- To phase, from **Process** select phasing and phase using the cursors at the bottom and then Keep. Phase corrected 1D spectrum will be displayed.

2D Spectrum

1. You will first need to change to **2Dmode**.
2. Under **user** find E-Z 2D transform, and then D1(t2) states or TPP.
   Enter the following manually in the pop-up window:

Input filename:	*name*
Data format:	new
Matrix name:	*name*.mat
Number of t_1 exps:	ni (for Varian)
Dimension 1 size:	1/2 * np
Dimension 2 size:	2^n value immediately larger than ni
DC offset:	yes
Fraction:	recommend 0.2
Current 1^{st} pt:	lpf
Solvent suppression:	as desired
Linear Prediction:	yes
Exponential filter:	select function (recommend exponential)
Window function:	select desired function

Transfer type:	complex
Phasing mode:	interactive
Phase 0:	0
Phase 1:	0
Fid to phase:	1
Baseline correction:	yes

3. Click on OK**.**
4. The program will ask for linear prediction and multiplier parameters at this point if you selected those options at this point. Choose variables as necessary, or keep the defaults.
5. Phase the 1D spectrum, which is displayed using the cursors at the bottom, and keep**.**
6. To Baseline correct Delete all points, and the auto peak FLATT. For a value of Basepoint Linewidth a recommended value of 11 may be used.
7. To apply correction, choose polynomial and then the order of the polynomial, and then Interval II and Exit.
8. Initiate Transform
9. If all has gone well, you can observe the transformation through the terminal window you used to open Felix.
10. Go to File and then open matrix.
11. Under **Display** draw intensity.
12. From **User**, now select EZ-2D-transforms and D2(t1) states.
    Window will pop up, and enter choices manually:

Correct 1st point:	lpf
Exp fill:	exp
Window:	choose as appropriate
Linear Prediction:	yes
Reverse vector:	yes
Phasing mode:	interactive
Baseline Correction:	yes

    Click on OK when done; the program will prompt you as before for Linear prediction and apodization function parameters.
13. For the 2nd dimension: use the default Spectral Width
14. For general Linear Prediction

1st pt :	1
Last pt :	your dimension size
Start point:	Dimension size + 1
End point:	as desired
# of coefficients:	64
Method :	Forward-Backward
Use root Reflection:	On
Type of mirror up:	90-180

    Click OK when done.

15. For 2D phasing, click on most upfield and most downfield peaks in the 1D spectrum displayed. Do the same as before for BC.
16. Initiate 2D transform.

To display 2D spectrum

1. Under **File**, open .mat file, and then **Display** Draw intensity.
2. Again, under **Display** plot parameters find data attributes. Choose attributes as desired, and then set.
3. Once again, **Display** and then Plot parameters general appearance Raw projection; adjust parameters as necessary. Finally, Draw.

To perform additional phasing

- Under **User** menu, find Rephase 2D matrix (and pick upfield and downfield peaks, and phase as usual).