Window Functions in 1D

NMR SPECTROSCOPY

(Xwinnmr for PC, versjon 3.5)

on

DPX 200, DPX 300, DRX 500

and

Processing computers

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Version I

Log in and start xwinnmr.

Manual Window Adjust is an interactive sub program in the Xwinnmr program where you almost instantly can see the effect of applying different window functions to a NMR spectrum (dataset). You are seeing the FID (free induction decay) and a visual representation of the mathematical function (window function) in the upper part of the screen and the effect of the function on the spectrum in the lower part of the window. **Winfunc** (also the name of the command to start the interactive display) is an extremely important tool when searching for the ideal function to apply to your FID. Winfunc is for instance a valuable tool when searching for small coupling constants in proton spectra.

1. Use one of your own data sets for this exercise.

2. Type **wrd**↵.

   Enter target data set **NAME:** **WINFUNC**↵ (or use your own expname)
   Enter target data set **EXPNO:** **1**↵ (use the expno seen in the top part of the xwinnmr window).
   Enter target data set **PROCNO:** **1**↵ (use the procno seen in the top part of the xwinnmr window).
   Enter target disk unit **DU**: **D:**↵ (if you want to, you can choose M: and the dataset will go to your home directory)
   Enter target user name **USER**: **uio user name**↵ (your own user name)

3. Use **search** to find the **WINFUNC** data set which is now owned by you, then **append** and **apply** it to the xwinnmr window and **efp** to Fourier transform it. You can not work properly with a dataset not owned or not processed by yourself. If the computer you are using does have another plotter attached than the one used under acquisition use **edo** (edit output) to select the new plotter. The data set does regretfully remember the plotter name connected to the computer used to acquire the spectrum.

4. **apk** the spectrum. Expand a sensible part (for instance 0.5 -3.5 ppm) of the spectrum on the screen and look at the form of the spectrum.

5. Type the command **winfunc**. Or go to Process followed by manual window adjust. The window splits in two. **FID** and **function** at the top and **spectrum** at the bottom.

6. The "command" buttons on the left hand side is divided in four sections, upper one = spectrum, second from top = fid, third from top = function: **EM** (exponential

multiplication), **GM** (gaussian multiplication), **sinm** (sine multiplication) and **qsin** (squared sine multiplication). The bottom section relates to parameters used by the selected functions.

7. Click on **ph-mod** and select **pk** to phase the spectrum.

8. In the small extra inf. window the current function and parameter is seen. For instance Window=EM, ph_mod = pk and LB (line broadening) = 0.3 Hz.

9. Work your way through different values of LB. LB 0, 1, 5 Hz for instance. Watch and remember the difference.

10. Select **GM** and see that the first part of The FID gets more importance and that fine structure in the spectrum does disappear at GB = 0. Change GB to positive values and watch the difference. Observe that the intensity of the resonances goes down as the GB goes up and the latter part of the FID gets a relatively higher importance.

11. Select **sinm** and SSB = 1 (where the starting point of the function is). Select SSB = 2. Observe the difference in S/N. Why does the S/N improve if the first part of the FID is given a lot of weight? Similarly play with different values of **qsin** and **SSB**.

12. Write down the parameters you want to use and select return and save and return. Open **edp** to select control the parameters. For instance **WDW = qsin** and **SSB = 1**. Type **qsin** and then **ft**. Observe that it is possible to select many more functions when clicking on WDW in the edp panel. To apply any of them use the name as a command followed by the ft command (not efp). Observe that sinm and qsin does give bad distortions on the baseline with negative peaks, but the added coupling constant information is often of high value in structure elucidation's.