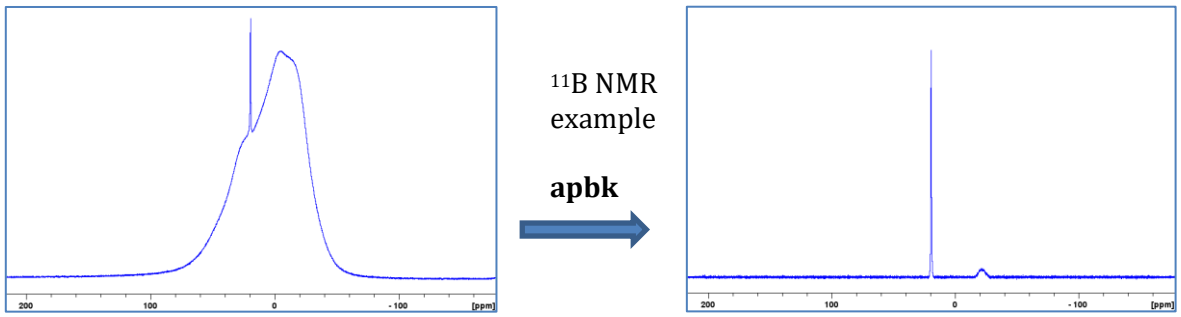
NMR Tips - Topspin Processing shortcuts

Bruker's Topspin has several commands that may help you speed up routine processing tasks. Some of these commands will only work (properly) in Topspin version 4.1 and higher.

Automatic phase and baseline correction: **apbk**

^{1}H, ^{13}C: improvement of poor phase correction
^{11}B, ^{19}F, ^{29}Si: flattening of broad background signals and baseline distortions

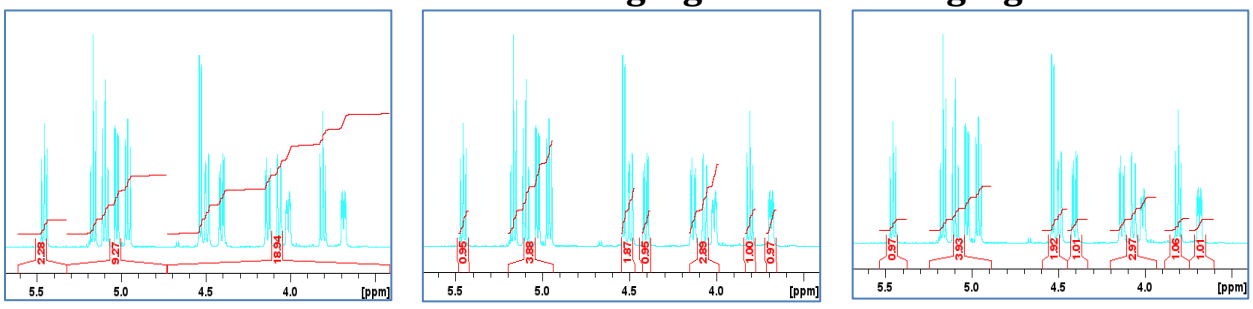


probe background (borosilicate glass) reduced background signal

Integration alternative: *presently for ^{1}H NMR only* **sigreg**

Before starting a manual integration, try:

automation default **sigreg** or **sigreg -add 30hz**



very narrow integrals wider integrals

Test sample: ***10 mM cellobiose octaacetate in $CDCl_3$***

SIGREG will only work with proton spectra.

Peak Picking: **pp**

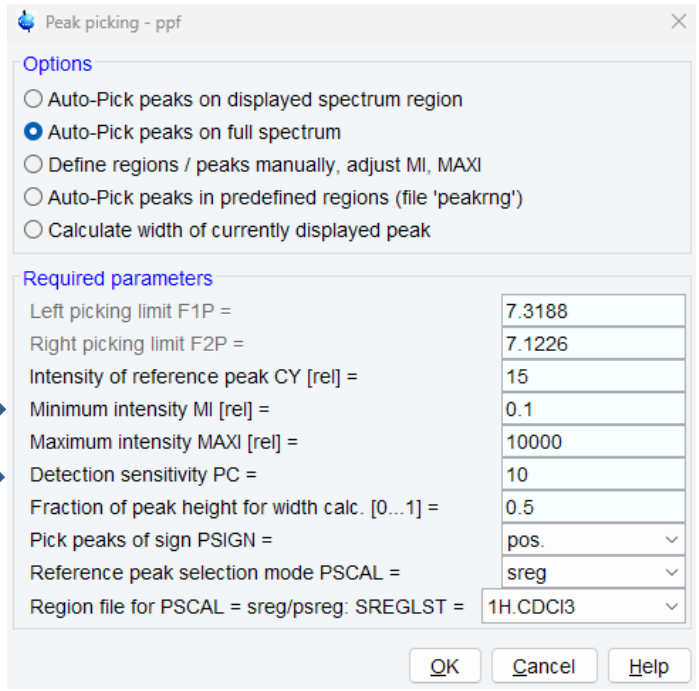
Type "pp" and change one or both of the following two parameters to determine the number of peaks to be picked:

Minimum Intensity MI:

- larger values will skip smaller peaks.
- smaller values will find smaller peaks.
  (in the noise between signals)

Detection Sensitivity PC:

- larger values will skip smaller peaks.
- smaller values will find smaller peaks.
  (within each multiplet)



First optimize **MI** to avoid picking empty regions. (= relative height of the smallest interesting peak)
Then optimize **PC** to adjust the number of peaks that are being picked above the MI level.

Calibration of any spectrum other than ^{1}H: **xiref**

Electronic chemical shift referencing is done mathematically with the IUPAC Xi scale.
This command requires an accurately calibrated proton spectrum of the same sample.
It also requires that all the spectra must be recorded in the same session as the ^{1}H spectrum.

1. Calibrate your ^{1}H spectrum using the signal of the solvent or of TMS (ideally).

2. Open your uncalibrated spectrum. Any experiment and any nucleus will work, i.e., COSY, NOESY, HSQC, HMBC, ^{13}C, ^{19}F, or any other nucleus.

3. Type the command "**xiref 10**" (assuming your ^{1}H spectrum is #10).

XIREF will allow you to accurately calibrate ^{13}C NMR spectra if your solvent is D_2O.
No additional internal or external standard is needed.