NMR Tips – Signal Apodization

The default settings of the NMR spectrometer's Auto-Processing routines have been selected to work with a wide range of samples. The resulting spectra may not yield all the information needed.

Apodization functions can be applied to your spectra to allow for better observation of ...
... small splittings by improving the resolution ... weak signals by increasing the sensitivity

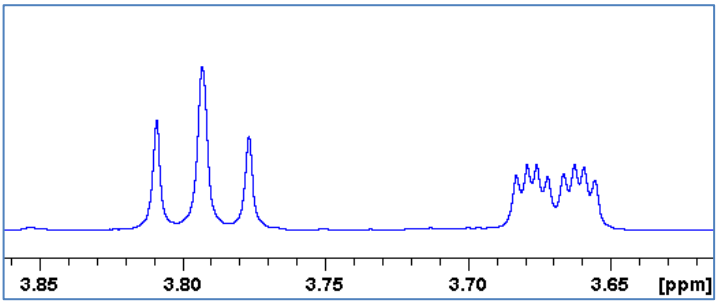
This is achieved by changing **LB** and/or **GB** in the "**Processing Parameters**":
A **positive LB** (Line Broadening) will broaden signals, a **negative LB** will sharpen them.
Setting **GB** between 0 and 1 will gradually change the line shape from Lorentzian to Gaussian.

<u>These data manipulations should always be reported when the data is published.</u>

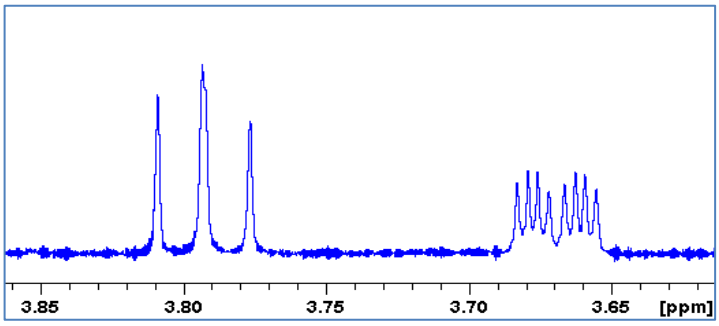
1. Resolution Enhancement

Small couplings can be better resolved in your spectra by applying a Gaussian window function.
You will gain resolution at the cost of sacrificing sensitivity and lineshape.

<u>Test sample</u>: 1 mM cellobiose octaacetate in $CDCl_3$

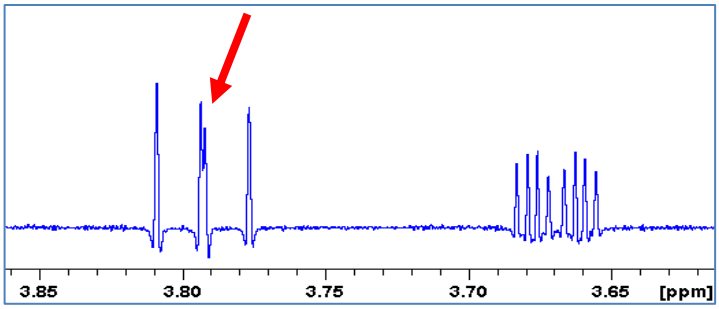


Spectrometer default settings.
Command: **FP**



LB = -0.5, Command: **EFP**

These moderate settings will allow for a more accurate measurement of small coupling constants ~1-2 Hz. (note the increased noise level)



LB = -2, GB = 0.4, Command: **GFP**

Choosing the more aggressive Gaussian function can resolve splittings < 1 Hz.
(see the marked signal)
As a trade-off, this will introduce severe distortions of the lineshapes.

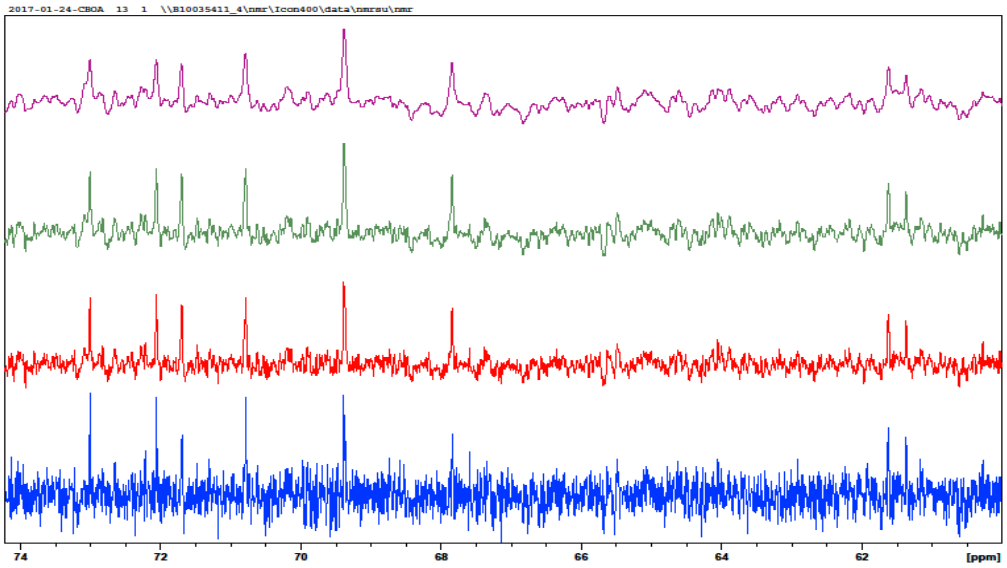
<u>Caution</u>: The signals can no longer be reliably integrated.

2. Sensitivity Enhancement

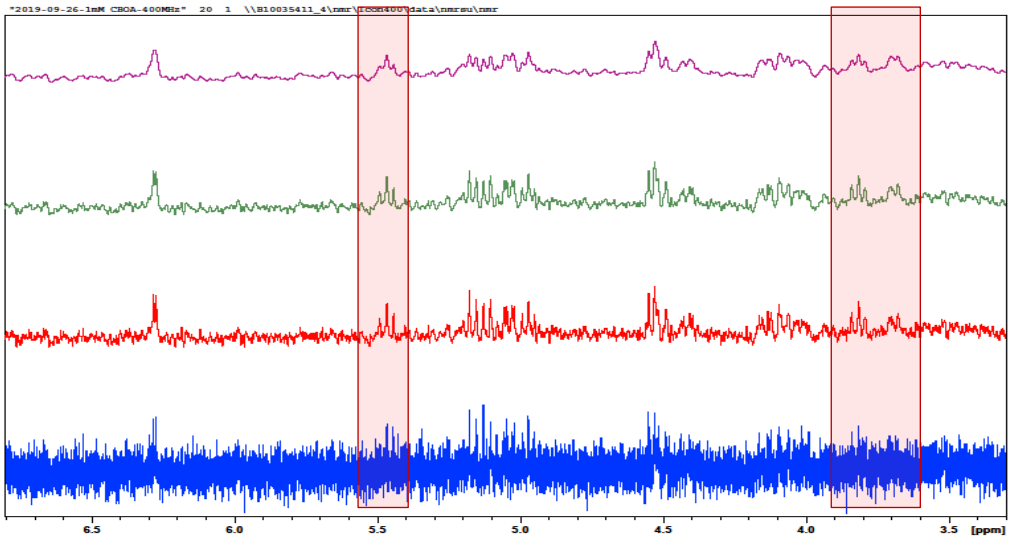
A poor signal-to-noise factor may make small signals (dilute samples) difficult to detect.
Line broadening is used to reduce the noise level of a spectrum, sacrificing some resolution.
My recommended settings: Processing parameters: LB = 1 or 2 (for ^{13}C)
Processing command: EFP

Test Sample: 1 mM cellobiose octaacetate in $CDCl_3$

In **^{13}C NMR** line broadening is routinely applied because of the low natural abundance of ^{13}C:



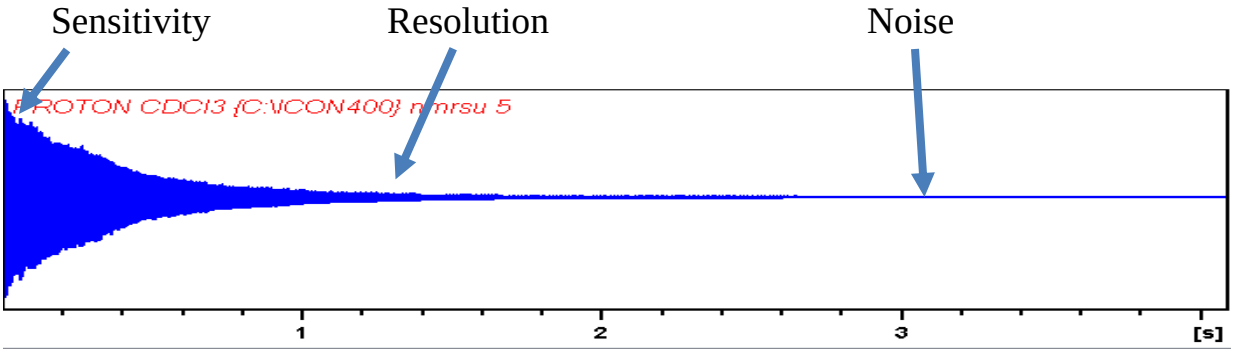
In **^{1}H NMR**, line broadening should only be used as a last resort to attempt finding weak signals:



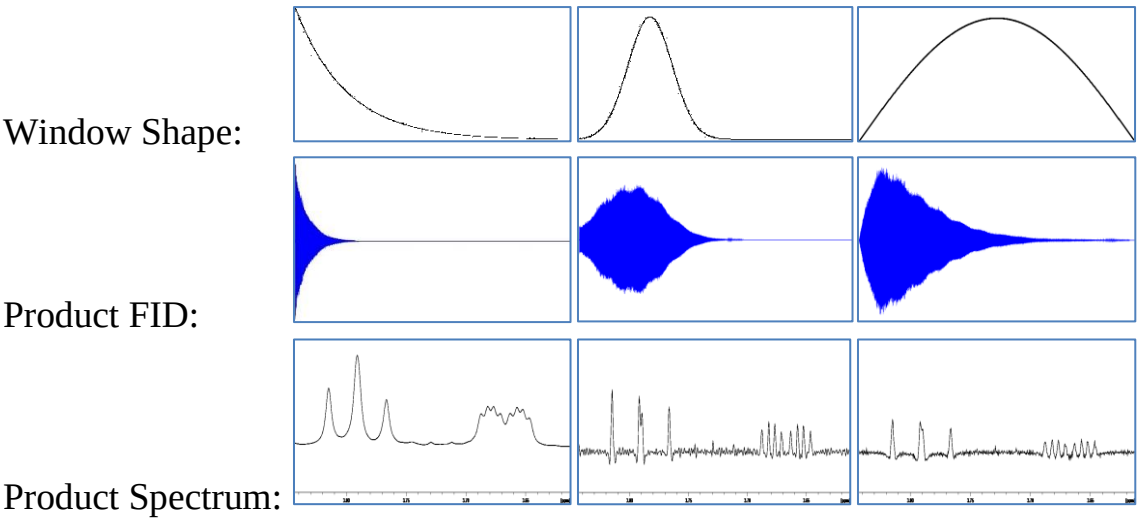
Choosing LB too large may merge signals or broaden signals beyond recognition.

3. How do Window Functions work?

Multiplying the raw NMR signal (*FID*) with selective window functions will emphasize certain features of the FID and suppress others:



Most frequently used window functions and their effects on the FID shown above:



Try the ***Interactive Window Multiplication*** in Topspin for spectrum optimization:

Open your spectrum, type **WM←** and select "**Manual Window Adjustment**".