V. Primer for Applying Pearson's Gaussian Apodization in DISNMR

[The following is taken directly from an e-mail message from G. Pearson, U. Iowa; see in addition the reference given below – revised 29-Oct-98]

A Gaussian apodization envelope works much better than an EM. For the same full width at half height, a Gaussian will have _much_ narrower feet than will a Lorenzian. The narrower feet mean that the "steps" in the integral will be significantly sharper, so the _height_ of the steps will be much better defined. Felix and Nuts (and presumably other off-line stuff) allow you to multiply by a Gaussian _WITHOUT_ necessarily multiplying by an increasing exponential at the same time, but the Bruker software incorrectly assumes that no one ever has any good reason to do just a simple Gaussian apodization.

You can lie to DISNMR and DISMSL so as to use a combination of GM and EM to produce a desired Gaussian broadening, without any Lorenzian garbage. Basic equations are in:

Gerald A. Pearson, "Optimization of Gaussian Resolution Enhancement", J. Magn. Resonance 74, 541-545 (1987).

In particular, eq. 11 gives the height of the shifted gaussian produced by GM, in terms of the intrinsic line width and the fractional sharpening which is wanted.

Let's take an example. Say you wanted to do a GAUSSIAN broadening of 5 Hz, and your acquisition time is 4.096 sec.

1. First, multiply by an envelope which will transform a 1-Hz Lorenzian into a 5-Hz Gaussian. [The 1-Hz Lorenzian is arbitrary, and will eventually cancel; you could use any other convenient LB.] By eq. 11:

   t_{max} = 2 ln2 / (π * 1 Hz * $(5/1)^2$)
   = 2 * .693 / (3.14 * 1 * 25)
   = 0.0176 sec.

   So you want to set

   LB = -1.0 and
   GB = (0.0176 / 4.096) = 0.00431

   and then do a GM.

2. Now, get rid of the increasing exponential:

   set LB = +1.0
   and then do an EM.

This is a real round-about way of doing such a simple thing, isn't it? That's one of the reasons why we [the Univ. of Iowa] routinely process stuff off line on a PC, using either Felix for Windows or NUTS (so use NUTS here at UW; if you are stuck with DISR, however, the above should help).