Generalized Lorentzian lineshape
with one new parameter for kurtosis fitting

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GSD – Global Spectral Deconvolution

f-domain algorithm which automatically decomposes sets of superposed (near) Lorentzians and ends up with a GSD Peaks List

Menthol at 750 MHz
The residuals comprise:

Systematic components (reproducible):
envelope of distinct transitions

Non-systematic components (irreproducible):
due to instrumental distortions shimming, decoupling, …)
Sources of peak-shape deviations from the Lorentzian shape

1. Magnetic field inhomogeneity (shimming)
2. Magnetic field noise
   (ebyte.it\library\docs\nmr06a\NMR_FieldNoise_Fid.html)
3. Sample spinning (ditto)
4. Sample temperature gradients (up to 0.01 ppm/deg)
5. FID weighting before FT (Voight and other profiles)
6. Distortions due to Discrete Fourier Transform (cyclic condition)
7. Overlap of miriads of transitions in coupled spin systems
8. Relaxation effects (e.g: methyls contain 3 transitions of different widths)
9. Molecular dynamics effects (chemical exchange, limited mobility)
10. etc …
Empirical (phenomenological) lineshapes

More fitted parameters
  => better peak approximation (always true)

Too many parameters
  => long execution times; convergence problems

Statistical correlation between parameters
  => big convergence problems, especially in the linearly swept mode used in GSD
Lorentzian - Gaussian mixing

Gaussian profile is unnatural (see Stan’s blog)
Plain linear LG combination implies two more parameters
Voight profile:
    Well justified, but only in some situations (LG apodization)
    Again two more parameters
In all LG approaches
    the new parameters correlate strongly with the old ones

Conclusion: LG mixing is not very good
The Lorentz property

\[ f(x) = 1 - \frac{1}{f(1/x)} \]

The physical meaning of this elegant mathematical property of the normalized Lorentzian line is not obvious. But it is nevertheless a good guiding principle.
Rational functions sharing the Lorentz property

For every rational order \((n \mid n+2)\) there exists a rational function which has the Lorentz property.

For \(n = 2\) one obtains a rational lineshape with a single variable parameter \(p\):

\[
L_p(x) = (1 - p)\frac{1}{1 + x^2} + p\frac{1 + x^2/2}{1 + x^2 + x^4}
\]
Generalized Lorentzian Lineshape Plots

The shape parameter in this graph ranges from –1.00 (blue) to +2.00 (red). For 0.00 (green), the line is a perfect Lorentzian.
Desirable properties of the new family of lineshapes

- Single extra parameter to be adjusted
- All members have the same position, height & half-height linewidth
- Hence: minimum correlation with the ‘old’ parameters
- The new parameter affects primarily the peak kurtosis

The Generalized Lorentzian lineshape is now operative in Mnova.

Users can configure their systems to use either the classical Lorentzian shape or the Generalized Lorentzian.
Example of the UI interface
Applications

✓ Improved quantitation of peaks
✓ Work in progress:
  Additional parameter for Auto-Edit
  (in particular for labile & water peaks scoring)
Thank You for your Patience

Any Questions?