Positive Probability Ltd

Note N1: NMR – Improving S/N

Introduction

Poor S/N is rarely a problem with modern NMR spectrometers. Even so, situations occasionally arise where it would be useful to improve the signal to noise ratio without broadening peaks. Unlike many modern mass spectrometers, NMR data acquisition hardware does not filter the data before it is presented to the user and the noise characteristics are generally very close to Gaussian.

In addition, NMR peaks are theoretically Lorentzian. The combination of Gaussian noise and Lorentzian peak profiles makes NMR data ideally suited to data reconstruction techniques and gains in S/N can be dramatic.

Data and Data Processing

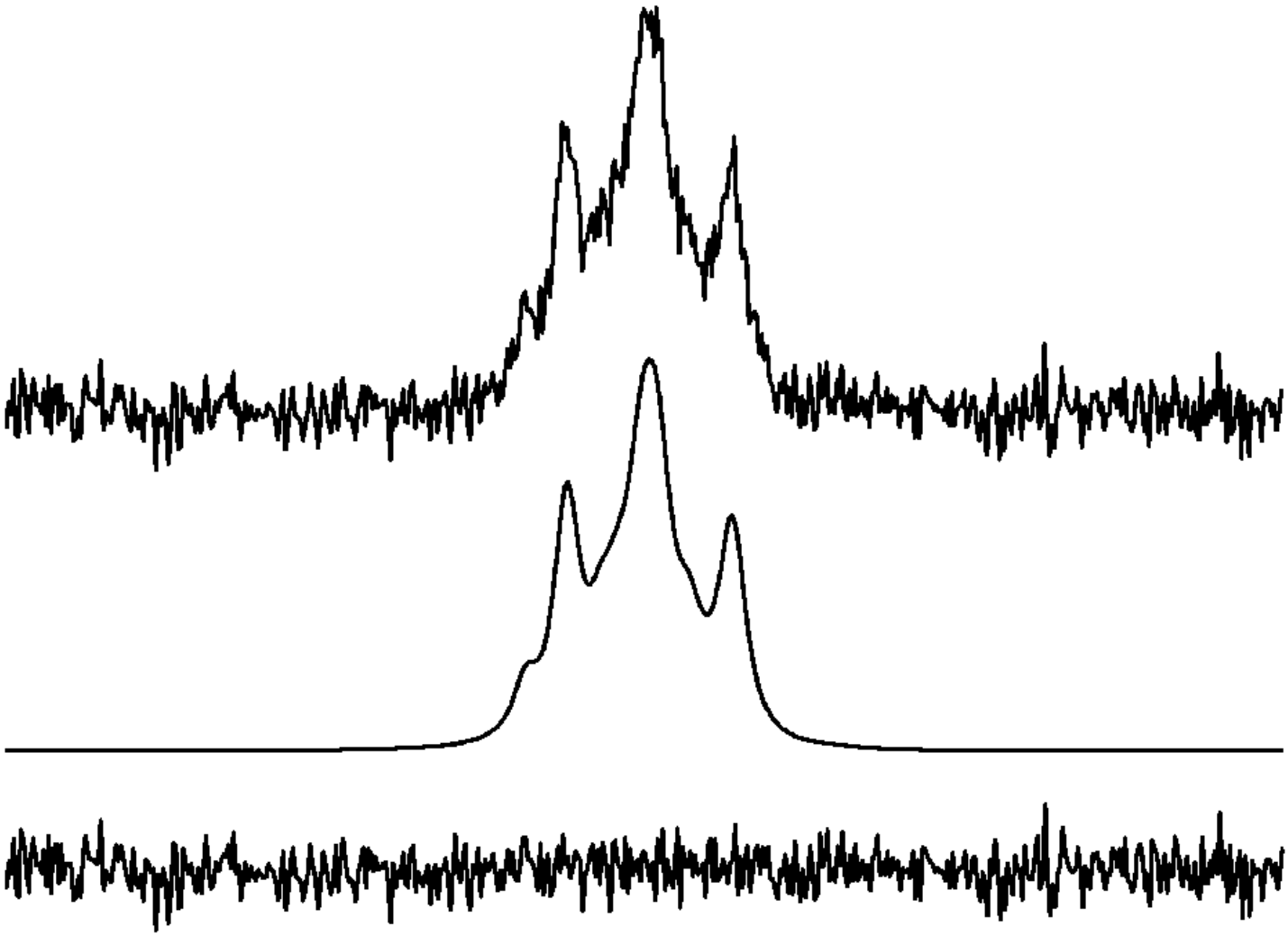
The data shown here are part of a 1H spectrum of a mixture of two optically active isomers that have been partially separated with an optically active chemical shift reagent. Each multiplet is a doublet of doublets with similar coupling constants so that the two central peaks of each multiplet are severely overlapped. The multiplets therefore appear to approximate to 1:2:1 triplets. The proportion of the two isomers is approximately 1:3 and, with such a poor S/N, it is difficult to see the minor component in the raw data without some imagination.

The data were processed using the fast S/N enhancement option. This is an option in the ***ReSpect***™–based ***Sleuth***™ deconvolution program and the only input was an estimate of the peak width. A compromise shape is automatically set and will provide excellent enhancements regardless of the actual peak shapes. For these data the peak width estimate was obtained from the peak at the right of the cluster of signals. The program is very tolerant of the input peak width and only a crude estimate is required. However, an estimate that is seriously too wide will cause peaks to be broadened. Also, an estimate that is much smaller than the true peak width will not provide the full potential gain in S/N enhancement.

Results and Discussion

The figure below shows the raw data, the reconstruction and the misfit. The reconstruction may be considered as a signal channel and the misfit as a noise channel. For these data the noise is truly random (Gaussian) and the signals and noise are separated very efficiently. It is now possible to clearly and unambiguously see the presence of the minor component in the reconstruction. A full deconvolution using the ***ReSpect***™–based ***Sleuth***™ deconvolution program reveals all the expected 8 peaks (results not shown).

Although NMR peak widths are dependent on the proton relaxation times, the variation is generally not excessive, apart from OH and NH signals. It is therefore generally possible to obtain very effective gains in S/N over the entire data range without broadening peaks. Unless the data are grossly over-sampled, such gains are not possible using linear Fourier filers. In addition, Fourier filters will always broaden peaks to some extent.



Top: Raw data; centre: reconstruction; bottom: misfit

Conclusions

This example demonstrates that signals may be very efficiently separated from noise, particularly when the data are unfiltered.