November 2021 NMR Topic of the Month: Signal-to-Noise

One Scan
S/N 149.2

Four Scans
S/N 301.9
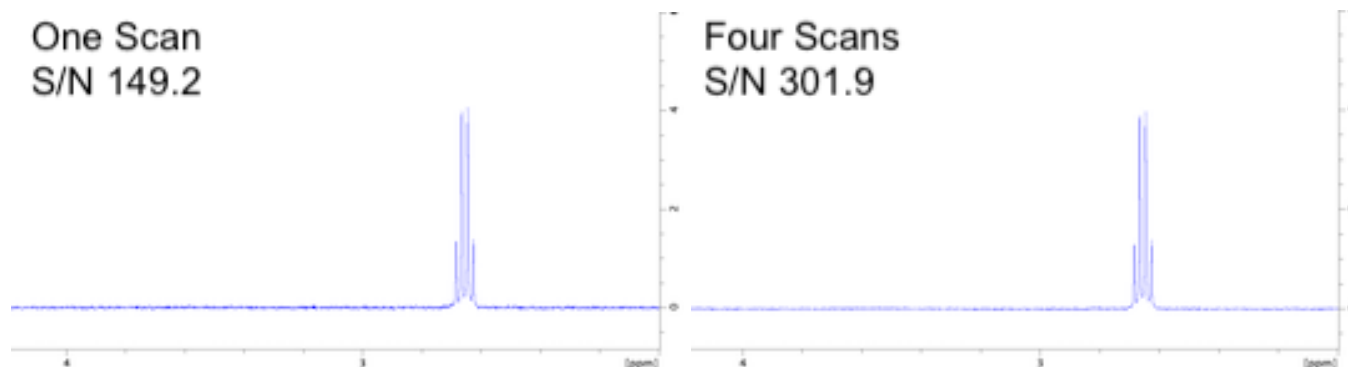
What is signal?

The response of the (entire) sample to the experiment. The signal should be constantly additive in the system response, which means the peaks of interest should get larger by the same amount for each transient. Mathematically, this means that the signal increases linearly with the number of transients (N), or $s_N \propto N$, and should not vary (zero deviation) between scans.

What is noise?

Usually, we mean random noise. Random noise is mean zero ($\mu=0$) with Gaussian (normal) distribution. Noise being random means that the noise is uncorrelated between data points ($\partial x_j / \partial x_k = 0$ if $j \neq k$). Mathematically, this means that an acquisition with N transients has a deviation that goes as:

$$\sum_{k=1}^{N} \sigma_k^2 \left(\frac{\partial \mu}{\partial x_k}\right)^2 = \sum_{k=1}^{N} \sigma_k^2 \left(\frac{\partial}{\partial x_k} \sum_{j=1}^{N} \frac{x_j}{N}\right)^2 = \sum_{k=1}^{N} \sigma_k^2 \left(\frac{1}{N} \sum_{j=1}^{N} \frac{\partial x_j}{\partial x_k}\right)^2 = \sum_{k=1}^{N} \sigma_k^2 \left(\frac{1}{N} N\right)^2 = \sum_{k=1}^{N} \sigma_k^2 = N\left(\frac{1}{N} \sum_{k=1}^{N} \sigma_k^2\right) = N\sigma^2 = \sigma_N^2$$

Therefore, the RMS value of the noise over N transients: $\sigma_N \propto \sqrt{N}$. Which means that the signal-to-noise $s_N/\sigma_N \propto N/\sqrt{N} = \sqrt{N}$. Which is why doubling a response's signal-to-noise on the same instrument requires four times the number of scans to acquire the original response.

Are there other kinds of noise?

Yes, they're far more obnoxious, and often called artifacts. There are a whole host of other annoyances that can interfere with your acquisition. They often are not mean zero and can sometimes be correlated. Let's be clear though, just because something is not a signal from your target molecule, that does not make it an artifact. For example, if you're doing a ^{11}B experiment and you use a standard boro-silcate tube, the large blob from the boron in the glass is not an artifact - it's a proper signal. However, you might sometimes see a response from the probe itself, which is a form of noise as it is not from the sample. There are often known methods for mitigating non-random noise.

How do I calculate the signal-to-noise in the software?

On a Varian system: expand the region of interest, then type "dsnmax(#)" on the command line, where # is the span of noise for comparison. On a Bruker system: type "sinocal" on the command line, and you will be asked to identify the frequency region containing the signal, a range of frequency without signal, and a frequency span within the noise range for comparison. Do not include the edges of the spectrum in S/N measurements because of filtering effects.

References

1. J.C. Hoch and A.S. Stern, *NMR Data Processing,* Wiley-Liss, New York (1996).
2. D.F. Mix, *Random Signal Processing*, Prentice-Hall, New Jersey (1995).
3. R.N. McDonough and A.D. Whalen, *Detection of Signals in Noise*, 2nd ed., Academic Press, San Diego (1995).