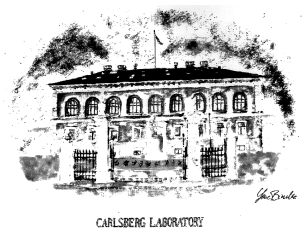
# Carlsberg Laboratory

*Danish Instrument Center for NMR Spectroscopy of Biological Macromolecules*




Prof. B.L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto CA 94303, **USA**

April 25, 2001

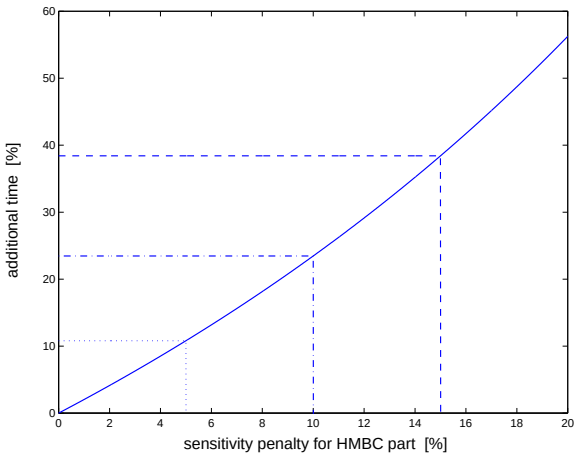
## How much sensitivity loss is acceptable in combined experiments?

Dear Barry:

Combining two NMR experiments into one in the sense that two different spectra can be extracted from the same data set is a potential spectrometer time saver. However, time saving can be deceptive if there is a penalty of reduced sensitivity for the combined experiment. The question is how much the sensitivity can drop before the apparent time saver becomes a time loser.

Let us by way of example consider combining HMBC and HSQC in the sense that a one-bond correlation spectrum can be extracted from an HMBC-type data set. HMBC is the least sensitive of the two so that is the experiment where the sensitivity is critical. Suppose there is a sensitivity penalty of x% for the HMBC part of the combined experiment. Then the combined experiment needs to run $\left(1-\frac{x}{100}\right)^{-2}$ times the time for the regular HMBC-type experiment in order to achieve the same signal-to-noise ratio. Of course, it is a bad deal if the added time exceeds the time it would take to record a separate HSQC spectrum.

The diagram to the right shows the additional time for the combined experiment as a function of the sensitivity loss of x% suffered for the HMBC part of the combined experiment. For example, "minor" sensitivity losses of x = 5, 10, or 15% requires that the combined experiment runs 11, 23, or 38% longer to achieve the same signal-to-noise ratio as in a separate HMBC-type experiment. The reference for judging the sensitivity in a spectrum should be the weakest signal of interest. Clearly, in order to estimate the practical value of a given combined experiment it is most helpful to know what its number x is.




The approach MBOB (Multiple-Bond and One-Bond correlation: *Magn. Reson. Chem.* **38**, 981-984 (2000); *The NMR Newsletter*, No. 508, January 2001; http://www.crc.dk/nmr/) for extracting a (broadband) HMBC spectrum and a one-bond correlation spectrum from the same data set is a full time saver as there is zero sensitivity penalty associated with this combined experiment.

Sincerely yours, Thomas Schulte-Herbrüggen Axel Meissner Ole W. Sørensen


Carlsberg Laboratory
Department of Chemistry
Gamle Carlsberg Vej 10
DK-2500 Valby, Denmark

Email: kbo@crc.dk
Email: jd@crc.dk
**Email: ows@crc.dk**

Tel.: +45 33 27 52 20
Tel.: +45 33 27 52 07
**Tel.: +45 33 27 52 09**
Fax : +45 33 27 47 08