High-resolution in 2D spectra using chemical shift encoding and spectral reconstruction

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High-resolution in the carbon dimension of 2D heteronuclear experiments, such as ^{1}H-^{13}C HSQC, has always been a problem because they are indirectly detected. Spectral aliasing [1] can be exploited by reducing the F1 spectral window, thus increasing resolution. The resolution enhancement factor is proportional to the reduction of the spectral window, within the same experimental time as a normal low-resolution spectrum. However, due to spectral aliasing, ambiguities in the chemical shift in the indirect dimension are introduced, making it difficult to determine their true chemical shift. Different methods have been reported to overcome these ambiguities [2,3].

We present here a generalisation of the chemical-shift encoding approach to resolve chemical shift ambiguities. The inclusion of an additional t_1' evolution time block, without quadrature discrimination, results in a signal splitting proportional to its ^{13}C chemical shift. Further processing allows a computer program to identify the partners for each peak splitting and calculate its true chemical shift based on the distance to the partner. Reconstructed full-width spectra are obtained by placing each peak at the position of its true chemical shift. The full and unambiguous reconstructed spectrum has the same resolution as the aliased spectrum, that is typically 10-100x higher than standard heteronuclear spectra.

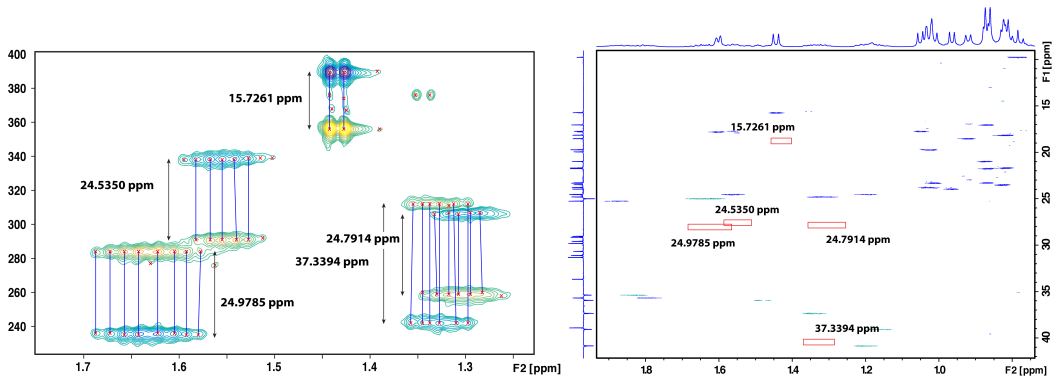

Figure 1. *(left) Example of an antiphase-splitted aliased edited HSQC spectrum with indirect dimension true chemical shift calculation. (Right) Expanded area of a reconstructed full-width edited HSQC spectrum. Highlighted signals correspond of the peaks shown on the left.*

[1] D. Jeannerat, Encyclopedia of Magnetic Resonance, John Wiley, Chichester, **2011**.
[2] Karla Ramírez-Gualito, D. Jeannerat, *Magn. Reson. Chem.* **2015**, 53, 901.
[3] M. Foroozandeh, D. Jeannerat, *Magn. Reson. Chem.* **2015,** 53, 894.