

Highly resolved pure shift NMR experiments for fast spectral assignment

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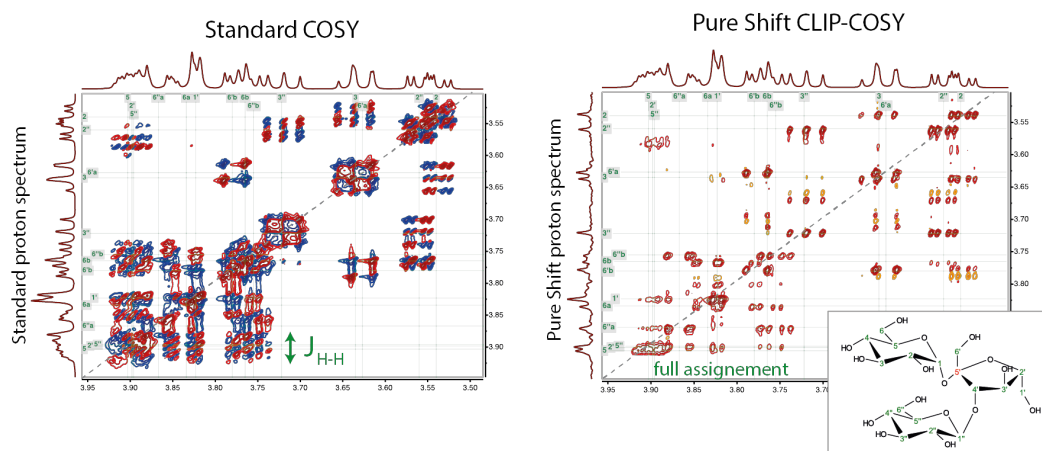
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The analysis of complex NMR spectra poses a real challenge for an organic chemist. Simplification and improved resolution of 1D and 2D proton spectra is highly desired to facilitate the spectral analysis hampered by severe signal overlap over a narrow range of chemical shifts. Recent developments in the NMR methodology provide an easily applicable solution that should facilitate the efforts of chemists seeking to structurally characterize their compounds.

Broadband homonuclear decoupling applied in the indirect dimension of a homonuclear 2D NMR spectrum leads to highly resolved pure shift proton spectra by collapsing the multiplets into singlets [1].

We present here a series of such experiments (2D DIAG [2], CLIP-COSY [3] and TOCSY [4]) with a singlet structure in F1 and multiplets containing the J-coupling information in the F2 dimension. The greatly increased information content of the spectra, relative to standard ¹H 2D experiments such as DQF-COSY will be demonstrated in the case of a mixture of carbohydrates.

The great interest in the development of the Pure Shift NMR methodology should equally impact the chemical community as it supplies modern, powerful tool, indispensable for structure elucidation of organic molecules and their mixtures.



[1] Juan A. Aguilar, Stephen Faulkner, Mathias Nilsson, Gareth A. Morris, *Angew. Chem. Int. Ed.*, **2010**, 49, 3901 – 3903.

[2] Axelle Cotte, Damien Jeannerat, *Angew. Chem. Int. Ed.*, **2015**, 54, 6016-6018.

[3] Martin R. M. Koos, Grit Kummerlowe, Lukas Kaltschnee, Christina M. Thiele, Burkhard Luy, *Angew. Chem. Int. Ed.*, **2016**, 55, 7655-7659.

[4] Klaus Zangger, Heinz Sterk, *J. Magn. Reson.*, **1997**, 124, 486-489.