Very long-range correlations (nJC, H n > 3) in HMBC spectra

Araya-Maturana, Ramiro

Pessoa-Mahana, Hernán

Weiss-López, Boris

The structural elucidation of natural products and complex organic molecules relies heavily on the application of proton detected heteronuclear NMR. Among these techniques, the HMBC NMR experiment remains as the most popular among the methods that sample long range coupling constants. The HMBC (C-H) experiment allows the assignment of structural fragments through correlations between protons and carbons separated by more than one bond, usually two or three (2JC,H and 3JC,H). It is also possible to obtain valuable information, sometimes crucial, through very long-range, or nonstandard correlations, nJC,H n>3; they can, surprisingly, appear in standard HMBC spectra, or looked for by performing several HMBC experiments with different long-range delays and using a deeper threshold in the contour plot.