

Use of long-range C-H (nJ $n>3$) heteronuclear multiple bond connectivity in the assignment of the ^{13}C NMR spectra of complex organic molecules

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The structural elucidation of complex organic molecules relies heavily on the application of proton detected heteronuclear NMR. Among these techniques, the HMBC NMR experiment is probably the most useful 2D NMR method. 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 bonds ($2J_{\text{CH}}$ and $3J_{\text{CH}}$) via ^1H , ^{13}C -coupling constants. It is also possible to obtain valuable information through longer correlations, nJ_{CH} $n>3$, performing several HMBC experiments with different long-range delays and using a deeper threshold in the contour plot. There have been several attempts to improve the results of the HMBC experiment, mainly focused on the question of optimization of the long-range delay, τ_2 . The D-HMBC, 3D-HMBC, CT-HMBC, ACCORD-HMBC, IMPEACH-MBC and CIGAR-HMBC experiments which provide much better experimental access to sample long-range couplings are briefly discussed. These