

NMR Methods for the Measurement of Small Heteronuclear Coupling Constants at Natural Abundance: An Overview.

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During the last decades many efforts have been dedicated to the design of NMR methods to measure small heteronuclear coupling constants in small sized molecules at natural abundance¹. A general overview describing the advantages and drawbacks of the most relevant NMR methods to measure them will be provided. We will start with a description of old carbon-detected, heteronuclear cross-polarization² or selective 1D³ experiments and their current potential use as complement tools to modern proton-detected 2D experiments. The most relevant aspects about features and performance of the state-of-the-art HSQC-TOCSY⁴ vs HMQMBC⁵ experiments will be discussed and the incorporation of spin state-selective methods and IPAP approaches will be evaluated experimentally and by simulation. Analogous time-shared NMR experiments⁶ will be also introduced as an opportunity for the simultaneous measurement of different proton-carbon and proton-nitrogen coupling constants.

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