

High-Resolution Two-Field Nuclear Magnetic Resonance Spectroscopy

Supporting information

Samuel F. Cousin,^{a,b,||} Cyril Charlier,^{a,b,||,†} Pavel Kadeřávek,^{a,b} Thorsten Marquardsen,^c Jean-Max Tyburn,^d Pierre-Alain Bovier,^e Simone Ulzega,^{e,§} Thomas Speck,^e Dirk Wilhelm,^{e,¶} Frank Engelke,^c Werner Maas,^f Dimitrios Sakellariou,^g Geoffrey Bodenhausen,^{a,b} Philippe Pelupessy,^{a,b} Fabien Ferrage^{a,b,*}

^aDépartement de Chimie, Ecole Normale Supérieure, PSL Research University, UPMC Univ Paris 06, CNRS, Laboratoire des Biomolécules (LBM), 24 rue Lhomond, 75005 Paris, France.

^bSorbonne Universités, UPMC Univ Paris 06, Ecole Normale Supérieure, CNRS, Laboratoire des Biomolécules (LBM), Paris, France.

^cBruker BioSpin GmbH, Silberstreifen 4, D 76287 Rheinstetten, Germany.

^dBruker BioSpin, 34 rue de l'Industrie BP 10002, 67166 Wissembourg Cedex, France.

^eBruker BioSpin AG, Industriestrasse 26, 8117 Fällanden, Switzerland.

^fBruker BioSpin, Billerica, Massachusetts 01821, USA.

^gNIMBE, CEA-CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France.

Low-field HSQC spectrum

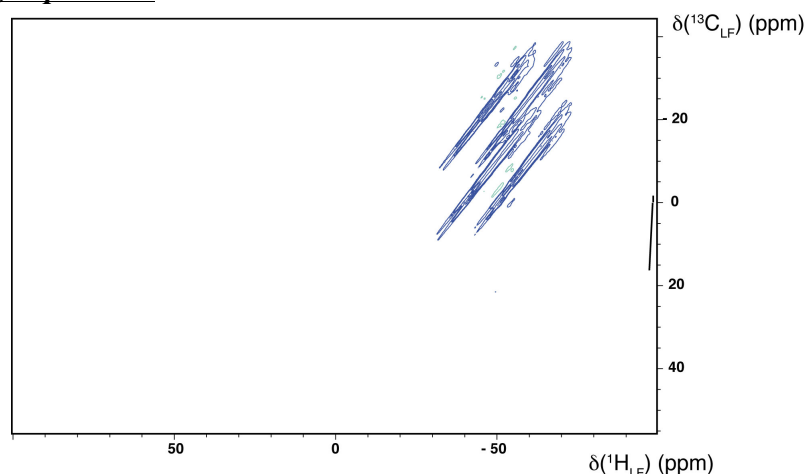


Figure S1. Two-dimensional low-field HSQC spectrum. After polarization of the nuclear spins at 14.1 T, the sample is transferred to the second magnetic centre at 0.33 T, where the pulse sequence is applied. The evolution in the indirect dimension and detection take place at 0.33 T. The multiplet pattern is similar to the one observed in the two-field HSQC. The scalar coupling $^1J_{\text{HC}} = 4.5$ Hz between the carboxyl $^{13}\text{C}'$ and the ^1H in glycine leads to a doublet in the horizontal direct ω_2 dimension. The homonuclear coupling $^1J_{\text{CC}} = 53.5$ Hz between $^{13}\text{C}^{\text{a}}$ and $^{13}\text{C}'$ leads to a splitting in the vertical indirect ω_1 dimension. In addition, the small scalar coupling between $^{13}\text{C}^{\text{a}}$ and ^{15}N may lead to a small splitting in the vertical indirect ω_1 dimension. This two-dimensional multiplet is convoluted with the magnetic field distribution function along the “diagonal”.

Comparison between 2F-INAZEQUATE and 2F-INADEQUATE spectra

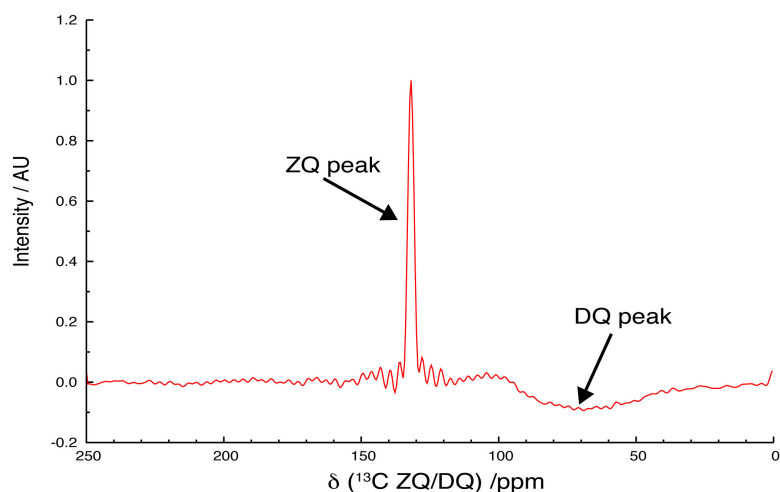


Figure S2. 1D slice extracted from 2D tow-field multiple quantum correlation where both zero-quantum and double-quantum coherences contribute to the signal. This is achieved by omitting the coherence selection pulsed field gradients at low magnetic field. This spectrum was recorded on a 1M solution of glycine (98 % enriched in ^{13}C , ^{15}N) in 97 % D_2O . The free induction decay was multiplied by an exponential apodization function (line broadening 5 Hz) has been used during the processing. The resolution of the 2F-INAZEQUATE spectrum is reduced due to a limited sampling of the time domain in the indirect dimension ($t_{1\text{max}} = 170.4$ ms).

Linearity of the low-frequency amplifiers

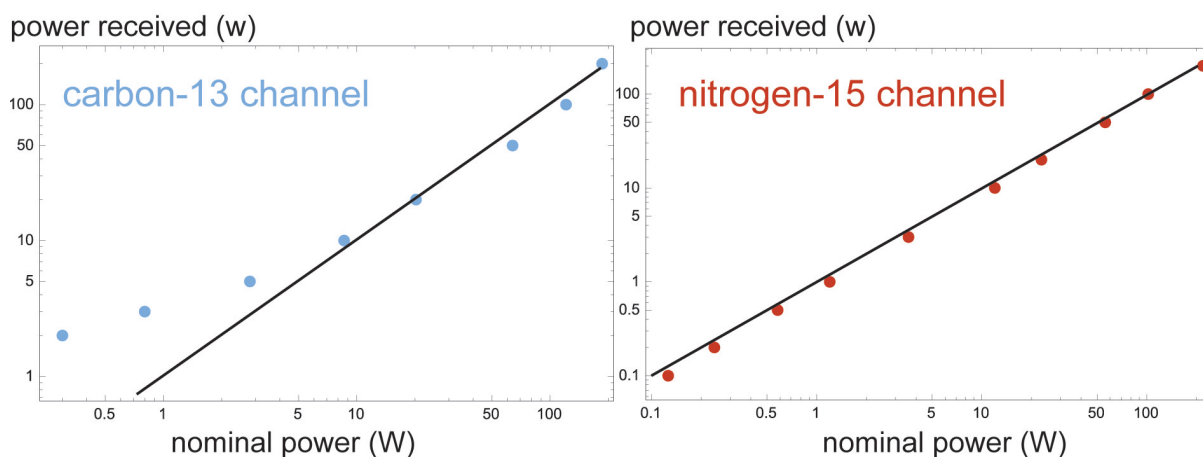


Figure S3. Measurement of the linearity of the low-frequency amplifiers employed on the carbon-13 and nitrogen-15 channels at low field.