A New Method for Localized Proton NMR Spectroscopy without Water Suppression Using Standard PRESS with and without Inversion of Metabolite Signals

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Introduction: Several methods have been published to realize localized in vivo proton NMR spectroscopy (MRS) without water suppression (WS) [1-6]. MRS without WS allows the water to be used as a reference for data correction during postprocessing and for absolute quantification without additional scans. While digital noise is of minor importance in modern NMR systems, despite the large dynamic range of the time domain (TD) data, gradient induced sidebands of the water signal are the major technical challenge for MRS without WS. To avoid these artifacts, 2D experiments or measurements with long echo time TE have been performed. For short TE MRS without WS, either the symmetry of the sidebands in the upfield and downfield region with respect to water has been used in additional postprocessing methods or the sign of the spoiler or all gradients has been inverted in two-step experiments. This study describes a new two-step method for MRS without WS: The simultaneously detected water and metabolite signals can be easily separated by adding/subtracting the TD data measured with a standard single voxel pulse sequence performed without or with additional chemical shift selective inversion of metabolite signals.

Method: The proposed method exploits the fact that the gradient induced sidebands originate from the narrow-band water signal, although they occur in a broad spectral range and overlap with many metabolite signals. The pulse sequence used for MRS without WS is shown in Fig.1. Prior to a standard PRESS [7] sequence, chemical shift selective inversion pulses are switched off (A) or switched on (B) in two consecutive experiments, yielding the TD data S_A and S_B. The inversion pulses followed by spoiler gradients invert the signals in the spectral range where metabolite signals are to be observed, either upfield or downfield with respect to water, but leave the water signal unaffected. Therefore, the water signal and the gradient induced sidebands come up in the same way in both TD signals (and the corresponding FT spectra). Thus S_A-S_B yields the metabolite signals with strongly reduced water signal and correspondingly reduced or even eliminated gradient induced artifact signals. S_A+S_B represents the water signal and can be used as a reference signal. To account for experimental imperfections of the inversion pulse, the TD signal S_B was scaled by a factor F_B to yield the same water intensity. Furthermore, possible B_0/frequency phase shifts were corrected based on a linear regression of the complex TD data of the first part of the FIDs.

Experimental: The pulse sequence was implemented on a 4.7 T Biospec system (Bruker, Germany) equipped with self-shielded gradients (170 mT/m, 450 µs). A saddle-type RF coil (98 mm i.d.) was used for homogeneous RF excitation/refocusing. The same coil was used for signal reception in measurements on a spherical phantom (37 mm i.d.) containing a solution of 50 mM N-acetyl aspartate (NAA) and 50 mM myo-inositol (Ins), whereas an 18mm surface coil was used for in vivo studies on healthy rat brain. The main sequence parameters were: voxel size: 5*5*5 mm^3 (phantom) or 4*4*4 mm^3 (*in vivo*); TE=18 ms; TR= 3, 6 or 15 s; 32 accumulations; 6 dummies; spectral width: 4006 Hz with digital filtering; 8K data points. To achieve a sharp transition between inverted and noninverted states, asymmetric adiabatic pulses were used as described by Hwang et al. with the following parameters using the nomenclature of [8]: [$HS_{1/2}$, R=31.415, $0.9 \cdot T_p$; tanh/tan, R=100; $0.1 \cdot T_p$], pulse duration T_p=12.5 ms, offset frequency: +/-336 Hz. The measured frequency profiles of the inversion pulses are given in Fig.2. As these inversion profiles have an asymmetric frequency profile, the pulses that invert the metabolite signals upfield and downfield from water exhibit an inverted phase evolution.

Results: Fig.2a-c depicts FT phantom spectra (TR=6 s) of (a) S_A and (b) S_B showing the same water signal and gradient induced artifact but inverted metabolite signals. The phase corrected FT spectrum of S_A-$S_B \cdot F_B$ is shown in Fig.2c demonstrating the excellent suppression of water and the gradient induced sidebands. Note that even the small NH signal of NAA at 8 ppm can be observed. Using the peak areas of the CH_3 signal of NAA and the water signal and a long TR of 15 s to avoid T_1 effects, the difference between the nominal and the measured absolute concentration of NAA was less than 3%. An *in vivo* spectrum of the rat brain acquired without WS is shown in Fig.2d, again calculated by FT of S_A-$S_B \cdot F_B$. Very good spectrum quality and high reproducibility is achieved despite the short TE of 18 ms. The spectrum quality in the range of 4-1 ppm is comparable with standard PRESS spectra (TR=6.0s, TE=18ms, NA=64) acquired with CHESS WS.

Discussion: To minimize T_1 and T_2 relaxation effects, the delay between inversion and signal excitation and the duration of the inversion pulses should be as short as possible. The latter is easily achieved at high B_0, but may cause increasing problems at low B_0 (small chemical shift in Hz). Note that only one inversion pulse is required if only signals from the upfield or downfield frequency range are of interest. Besides adding one or two adiabatic RF pulses followed by spoiler gradients, the new method for MRS without WS requires neither any modifications or adjustments of the pulse sequence nor any sophisticated data postprocessing.

Conclusion: A new two-step method for MRS without WS is presented in which optimized chemical shift selective inversion of metabolite signals is applied or not applied prior to a standard PRESS sequence. The method is easy to implement and does not require any additional experimental adjustments or specific postprocessing schemes. As this approach can also be used for other single voxel or spectroscopic imaging (SI) methods, it should be widely applicable to ^{1}H MRS or SI without WS.

References: [1] Hurd RE et al., Magn. Reson. Med. 40, 343-347(1998). [2] Kreis R, Boesch C, Proc. ISMRM, Sydney, 1998, p.24. [3] van der Veen JW et al., Radiology, 217, 296-300(2000). [4] Serrai H et al., J. Magn. Reson. 149, 45-51(2001) and J. Magn. Reson. 154, 53-59(2002). [5] Clayton DB et al. J. Magn. Reson. 153, 203-209(2001) and Concepts in Magn. Reson. 13, 260-275(2001). [6] Dong Z et al., Proc. ISMRM, Honolulu, 2002, p. 2198. [7] Bottomley PA, Ann. N.Y.Acad.Sci. 508, 333-348(1987). [8] Hwang T-L et al., J. Magn. Reson. 138, 173-177(1999).

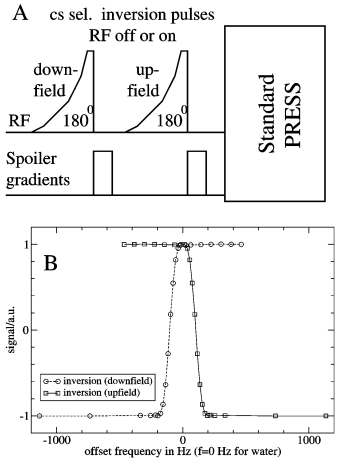

Fig.1: (a) Pulse sequence of the proposed two-step method for MRS without WS. (b) measured frequency profiles of the inversion pulses.

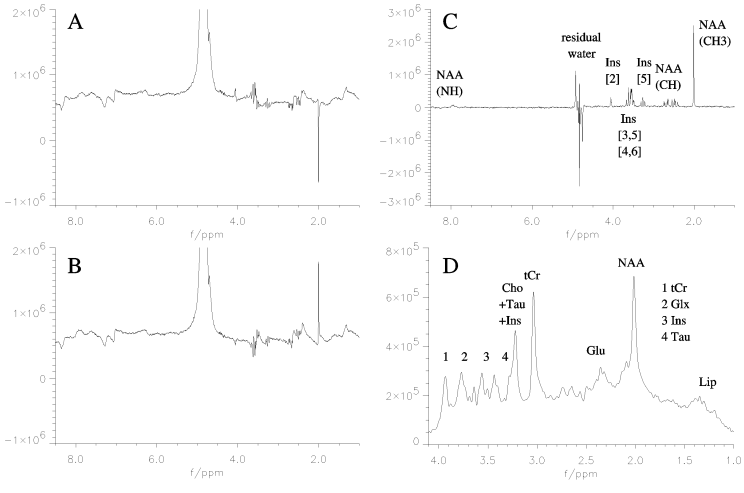

Fig.2: (a-c) Phantom spectra measured (a) without (S_A) and (b) with (S_B) chemical shift selective inversion of metabolite signals. (c) phase corrected FT spectrum of S_A-$S_B \cdot F_B$ (F_B=1.02). (d) in vivo rat brain spectrum (TE=18 ms) acquired without WS (FT(S_A-$S_B \cdot F_B$) with F_B=1.1).