New methods for the correction of ^{31}P NMR spectra in *in vivo* NMR spectroscopy

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The chemical shift imaging (CSI) NMR spectroscopy is widely employed in *in vivo* ^{31}P MR spectroscopy, since it enables simultaneous acquisition of data from multiple voxels (1 - 6). However, for some physical (short T_2 of many ^{31}P metabolites) and technical (high RF power demands) reasons, 180° pulses cannot be used for refocussing the chemical shift induced dephasing which arises during the phase encoding period prior to data acquisition. This results in the loss of the first few data points. Owing to their different precessional frequencies, the various resonances dephase at different rates during the time delay. For each dwell period during which the data collection is delayed, the total first order error increases by 2π radians. To compensate the phase error, it is much more convenient to shift, before the Fourier transformation, the acquired FID signal by an appropriate number of data points to the right. However, the spectrum obtained from the FID signal with missing several early data points is, as a rule, considerably distorted. Often, this distortion makes a reliable quantification of the obtained spectra absolutely impossible. A great effort is therefore devoted to the development of methods suitable for the correction of baseline distortions in *in vivo* CSI NMR spectra. The baseline distortion problem in CSI is dealt with in either the time or the frequency domains. Many sophisticated correction techniques belonging to both these categories have been developed until now, however a reliable solution to this problem has not been presented yet.

In this communication, we present a method for the baseline correction of ^{31}P NMR spectra which represents a combination of time-domain and frequency domain techniques. The basic steps of this technique are as follows: (a) The FID signal is acquired with the acquisition parameters adjusted so that the linear phase correction need not be performed (there are several zero data points at the beginning of the FID signal). (b) The obtained FID signal is multiplied by two knowledge-based line broadening functions, one related to the widths of ^{31}P signals in the spectrum (FID^A) and the other to the bandwidth of the spectral region of interest (FID^B). (c) Both FID^A and FID^B signals are Fourier transformed, giving spectra S^A and S^B (The spectrum S^B approximates the coarse baseline roll artifacts). (d) The spectrum S^B is subtracted from the spectrum S^A. (In this step, already a well looking spectrum can already be obtained). (e) The COBALD technique (7) is applied to the difference (S^A - S^B) spectrum (This method enables one to reconstruct the early data points in the FID signal from the difference spectrum. In this step, an appropriate choice of reconstruction parameters makes it possible to modify the resolution and the signal-to-noise ratio in the spectrum. If necessary, more iteration COBALD steps can be employed. The correction technique proposed is illustrated in Fig. 1. The starting ^{31}P spectrum processed as desired was obtained by measuring the snail in a 4.7 T NMR spectrometer.

Conclusions

The technique presented in this communication can be used with advantage for a very fast and efficient minimization of baseline artifacts is ^{31}P NMR spectroscopy of intact biological tissues. It can be estimated that, if fully automated, the technique proposed might enable one to accomplish the correction in times less than 1 s using some of standard

workstations. Even with some operator intervention, when this is considered necessary, the correction can be made in several minutes. The correction routine mostly utilizes the information contained in the starting spectrum. It does not use calculations based on a rigid mathematical formula describing a specific lineshape and as such it can be implemented on spectra of arbitrary appearance. The method is fairly robust and accurate and can be used quite successfully even at low signal-to-noise ratios.

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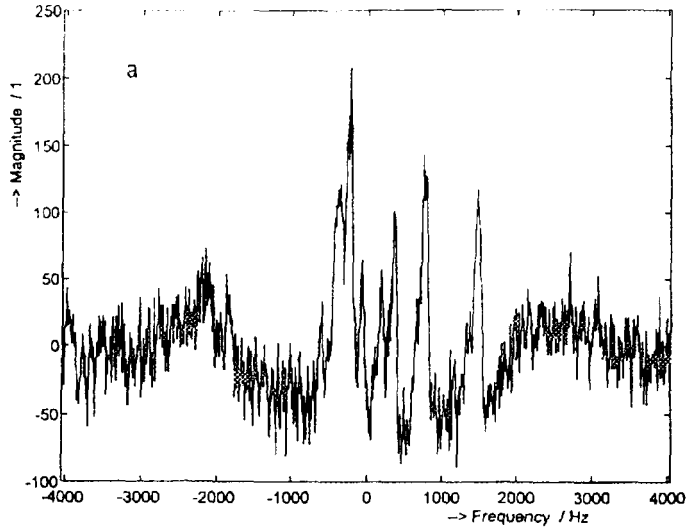
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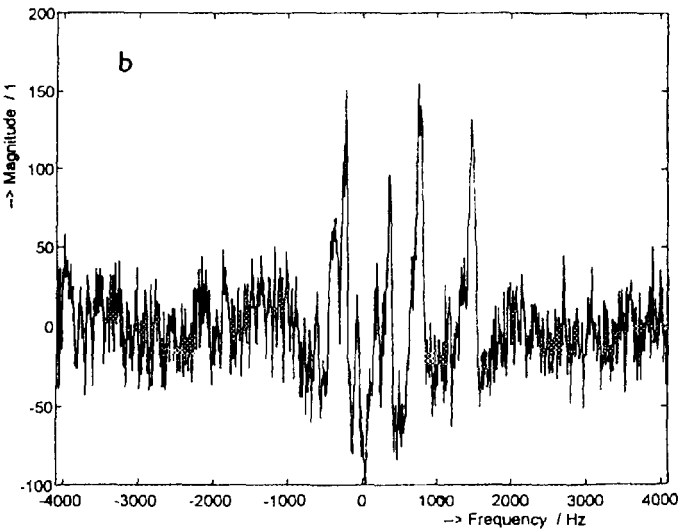
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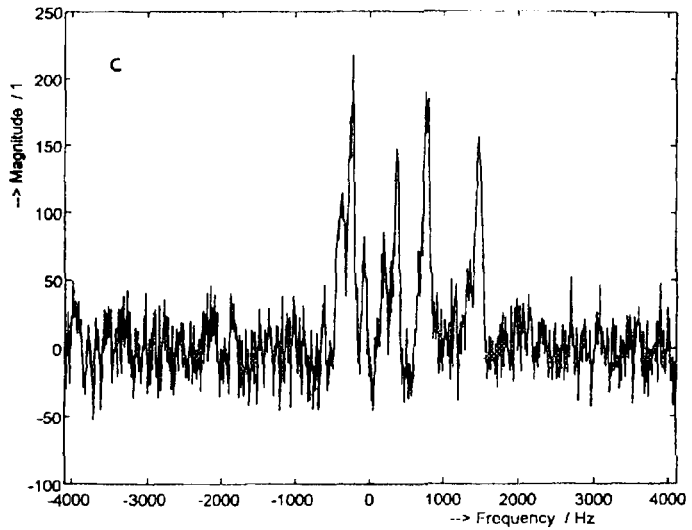

Fig. 1. Correction of the baseline in the ^{31}P NMR spectrum obtained from a snail at 4.7T.

(a) The original spectrum distorted due to missing early data points in the FID signal.

(b) The difference spectrum obtained as described in the text.

(c) The final spectrum obtained from the difference spectrum using a COBALD technique. Two iteration COBALD steps were employed.