

# Hadamard encoded iMQC high-resolution NMR spectroscopic method in inhomogeneous fields

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## Introduction

Intermolecular multiple quantum coherences (iMQCs) possess numerous interesting properties and have been developed rapidly for many important applications in magnetic resonance spectroscopy and imaging [1]. In the previous report, iMQCs have been applied to achieve 1D and 2D high-resolution NMR spectra in inhomogeneous fields via 2D and 3D acquisition. In this work, a new iMQC method involving Hadamard encoding [2] is proposed to obtain 1D NMR spectrum in inhomogeneous fields. It focuses on the chemical shifts while disregarding potential effects of spin-spin couplings. Spectra with relatively high-resolution can be obtained through 1D acquisition, which greatly reducing the acquisition time. The line-width can be greatly reduced. This method offers a new way to obtain high-resolution NMR spectra in inhomogeneous fields.

## Methods

The pulse sequence utilizes intermolecular double quantum coherence is shown in Fig. 1. The first pulse is a soft polychromatic pulse. Since the spectral line-width will be greatly increased in large inhomogeneous fields, we divide the solvent peak into  $N$  segments ( $N$  is the order of the Hadamard matrix), each has its own center frequency. These center frequencies are then encoded according to a Hadamard matrix to generate the soft polychromatic pulses. After  $N$  scans, the corresponding  $N$  composite responses are decoded by reference to the same matrix. Distant dipolar field takes effect after the action of the third RF pulse. Since the iMQC signals are only affected by the field inhomogeneity within the dipolar correlation distant instead of the whole sample, we can get solute signals with high resolution. In addition, the signal-to-noise ratio is increased by  $\sqrt{N}$  times due to  $N$  scans.

## Experiments and Results

Experiments were performed on a Varian NMR System 500 MHz spectrometer. A sample of butyl bromide and DMSO dissolved in chloroform was tested in an intentionally deshimmmed inhomogeneous field (300 Hz linewidth). Fig. 2(a) shows the conventional 1D spectrum in homogeneous field. An inhomogeneous field with a linewidth of 300 Hz was then achieved by deshimming the X1 and Z1 coil. The conventional 1D spectrum in this inhomogeneous field is shown in Fig. 2(b). In the same inhomogeneous field, an iDQC Hadamard experiment was carried out. The result is shown in Fig. 2(c). The acquisition time is about 2 min and the line-width of decoded spectrum reduces to 16 Hz.

In addition, a mouse brain phantom was used to testify the feasibility of the pulse sequence to more complicated spin systems. The sample was a H<sub>2</sub>O solution of 11 different brain metabolites [3]. The experiment result is shown in Fig. 3. The spectral line-width is reduced from 280 Hz to 21 Hz and the nearest two peaks become distinguishable.

## Conclusion

A pulse sequence employed Hadamard encoding technique was designed to fast obtain high-resolution 1D NMR spectra in inhomogeneous fields. It can not only recover spectral information concealed by inhomogeneous line broadening, but also greatly improve the resolution and signal-to-noise ratio of the spectrum within a relatively short acquisition time. It is effective to both simple and complex systems. Improvement of the sequence and optimization of experimental parameters may make it applicable to *in vivo* MRS studies.

## Acknowledgements

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## References

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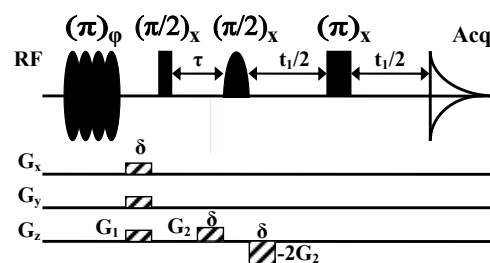


Fig. 1 Hadamard encoding iDQC pulse sequence

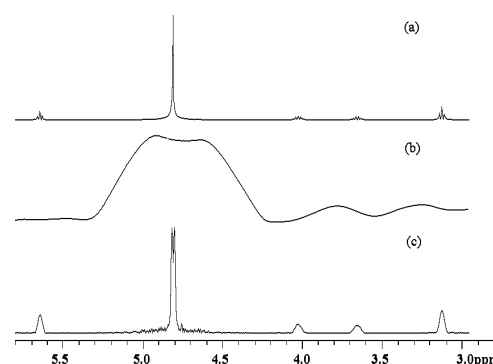


Fig. 2 1D NMR spectrum of the mixture of butyl bromide and DMSO in chloroform. (a) Conventional 1D spectrum in homogeneous field; (b) Conventional 1D spectrum in inhomogeneous field; (c) Hadamard encoded iDQC 1D spectrum in inhomogeneous field.

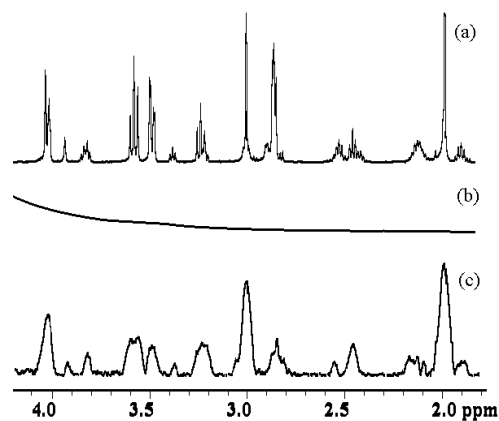


Fig. 3 1D NMR spectrum of the mouse brain phantom. (a) Conventional 1D spectrum in homogeneous field; (b) Conventional 1D spectrum in inhomogeneous field; (c) Hadamard encoded iDQC 1D spectrum in inhomogeneous field.