Theoretical and experimental studies of 2D J-resolved spectroscopy of GABA

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Introduction

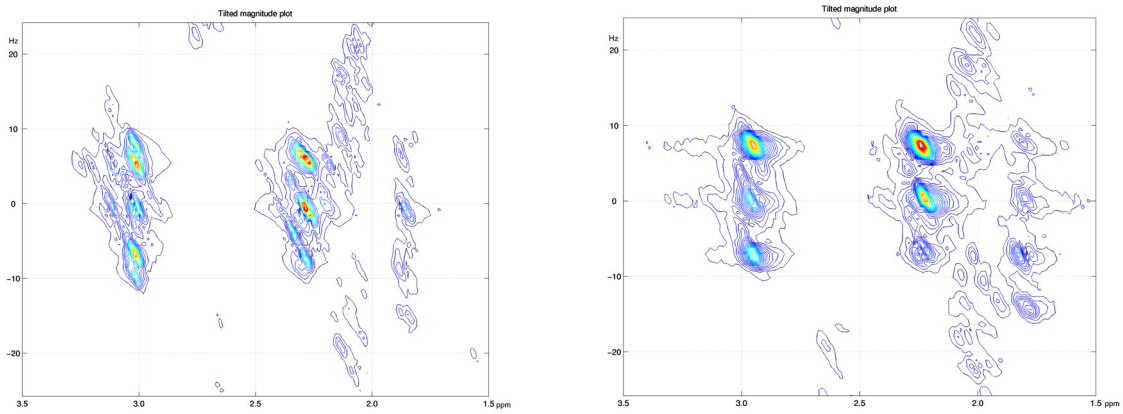
GABA is an important neurotransmitter that exhibits strong J-coupling at clinical field strengths. Its resonances are also overlapped by those of creatine and glutamate/glutamine, making in vivo detection very difficult. Spectral editing (1) and 2D J-resolved techniques (2,3) have been used. The former are technically demanding and have low detection efficiency. 2D J-resolved spectroscopy is simpler to implement, but there is little theoretical work on what the resulting 2D spectra should look like. In particular, we found asymmetries in experimental spectra that were not predicted by simple theory. We therefore carried out detailed simulations for comparison with experimental results.

Methods

Spin simulations were implemented using the GAMMA software package (4), with the chemical shift and J-coupling constants taken from the literature (5). The resonant frequency was set to 64 MHz (1.5T). We modelled the asymmetrical PRESS J-resolved sequence available on our scanner, with a fixed 10ms interval between the excitation pulse and the first refocusing pulse. To mimic physical experiments, we used 64 echo times with an incremental delay ΔTE of 10 ms. Non-ideal flip angle distributions were taken into account by summing sub-voxel signals over the volume of interest. Relaxation effects were ignored. *Experimental* 2D J-resolved spectra were acquired at 1.5T from a 100mM aqueous solution of GABA using a GE scanner fitted with the standard head coil. The PRESS-localised double spin-echo sequence was used to acquire FIDs from a 30 mm cubical volume of interest at the centre of the phantom. Timing details were as used in the simulations. *FID data* from both simulations and experiments were apodised, Fourier transformed and displayed in identical ways.

Results and discussion

The figure shows the simulated (left) and experimental (right) 2D spectra. The main features are clearly predicted, notably the triplets at 3.0ppm and 2.3ppm (shifted by 0.1ppm in the room temperature phantom), and the complex strong coupling peaks in the region 2.2-1.7ppm.



Asymmetries along the F1 (vertical) direction are readily apparent, and were caused primarily by non-ideal values of the second refocusing pulse.

Conclusion We have established a framework for investigating complex 2D spectra, and have successfully applied it to GABA.

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References 1. Keltner MRM 1997, 37:366-371; 2. Ryner MRI 1995, 13:853-869; 3. Ke Psych Res Neuroimag 2000, 100:169-178; 4. Smith JMR(A) 1994, 106:75-105; 5. Govindaraju NMR Biomed 2000, 13:129-153.