Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

High-resolution magic-angle spinning NMR metabolic profiling with spatially localized spectroscopy under slow sample spinning

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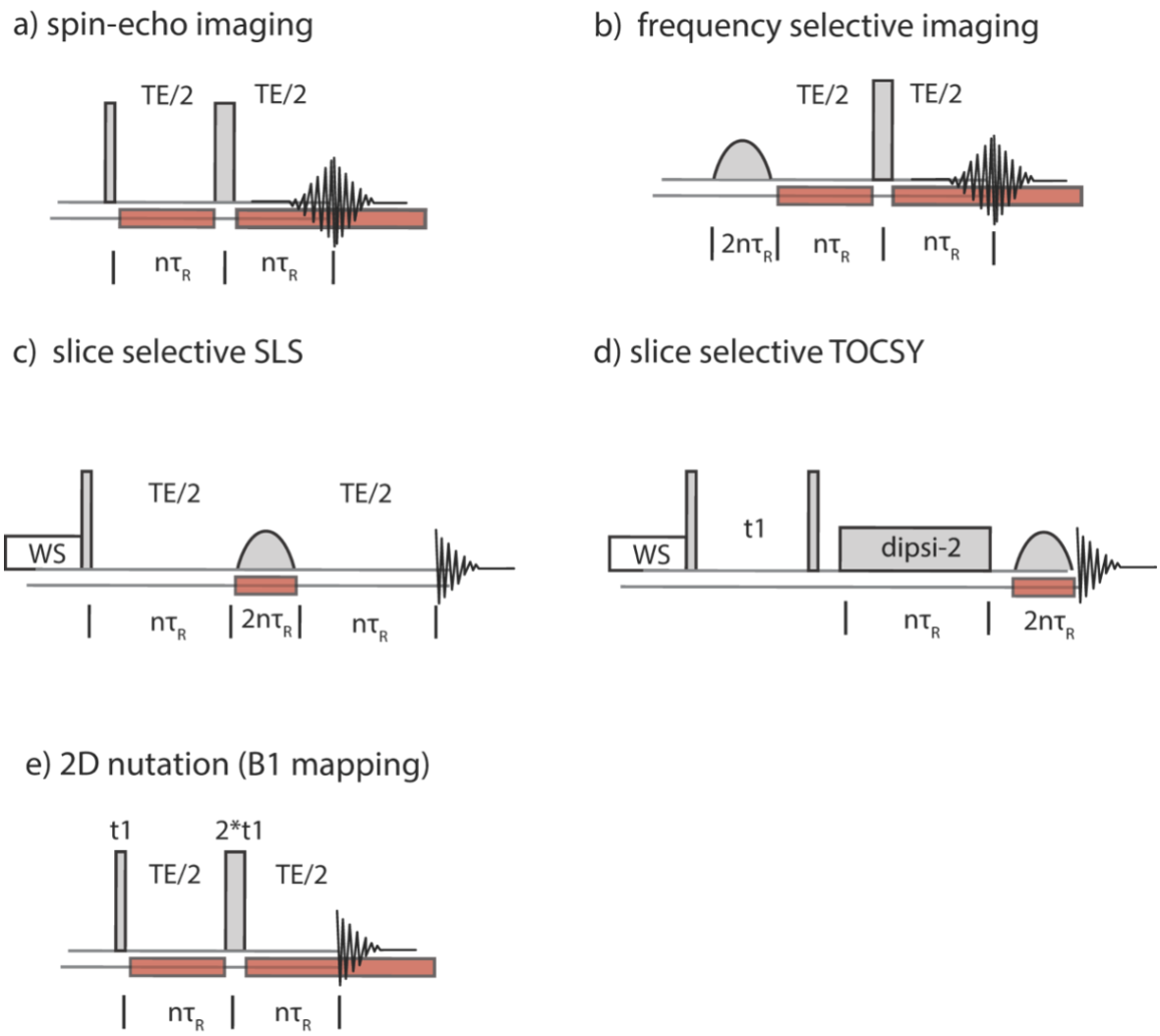

Figure S1. Pulse sequences used in the study: TE=total echo time and $n\tau_R$=rotor-synchronized cycles. A rotor-synchronized 4 ms shaped pulse was applied in all selective pulses sequences in (b,c,d) with MAS rate at 500 Hz or 4000 Hz. Slice selective TOCSY sequence was modified from a Topspin 'dipsi2phpr'. Nutation experiment was acquired with a half-echo acquisition. Experimental details can be found either in the text or figure caption.

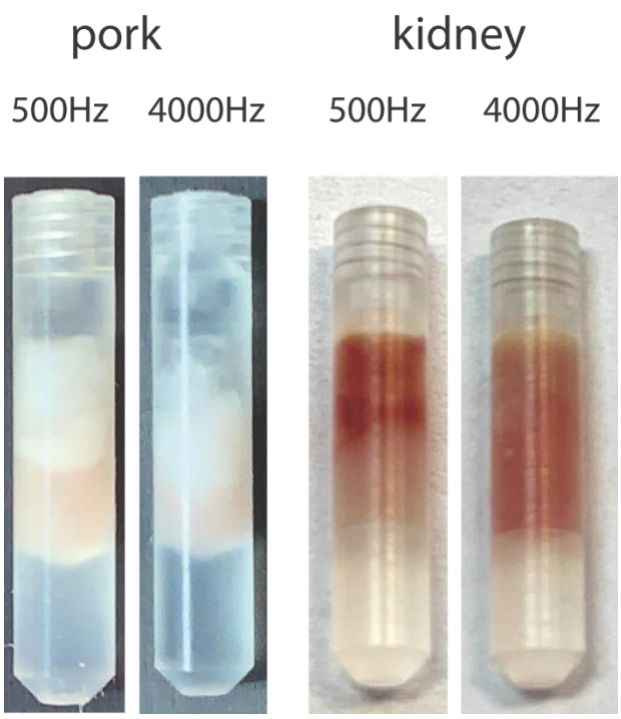

Figure S2. Photographs were taken after the MAS experiments, spinning at 500 Hz and 4000 Hz. The effect of the spinning is evident.

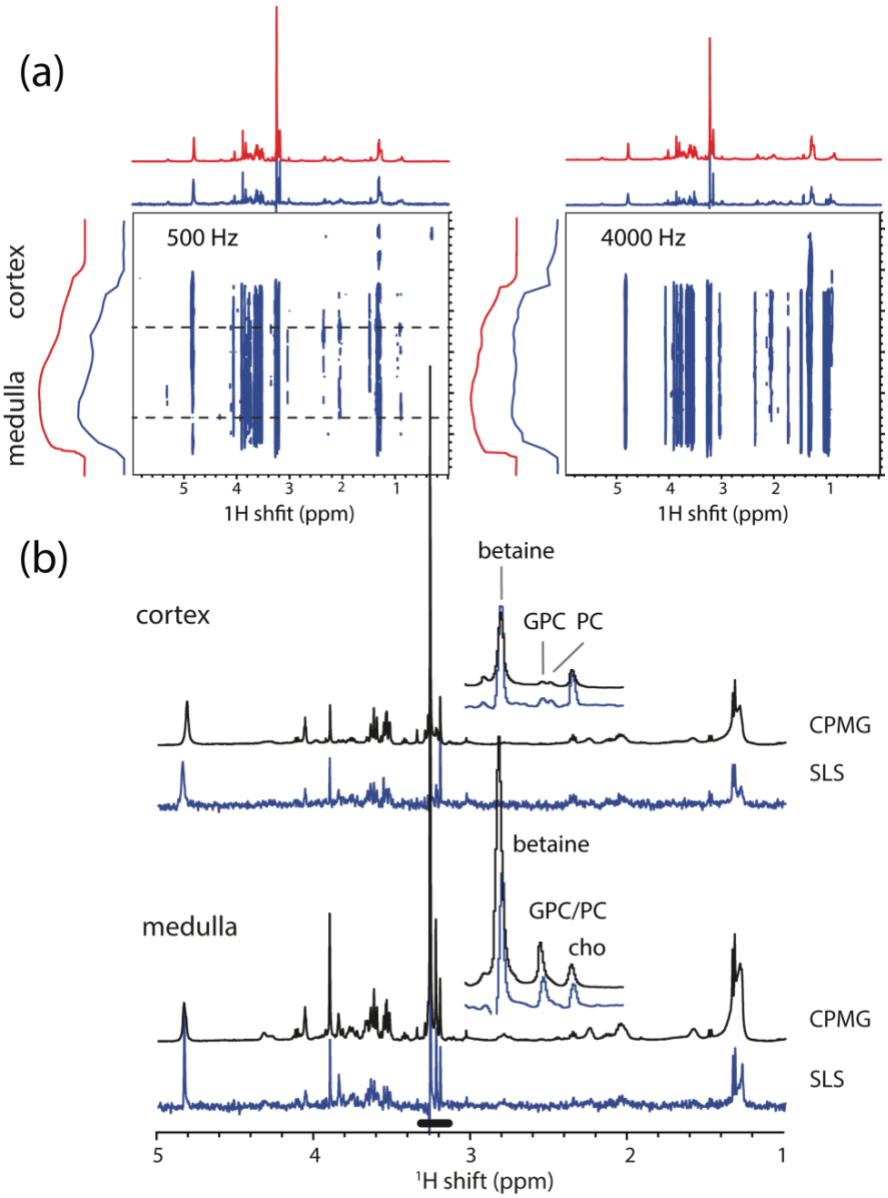

Figure S3. (a) 2D SLS spectra acquired with MAS at 500 and 4000 Hz. The F1 and F2 projections are shown in blue, and are found similar to corresponding CPMG spectra and images in red. The 2D SLS spectra were acquired by a succession of 1D SLS with 32 frequency shifting (32t1) with an offset increment of 2000 Hz; and each SLS were acquired with 32 scans and a 2 s recycle delay. The total acquisition time of the 2D SLS was 34 minutes. The slice selective pulse was composed of a 4 ms refocusing Rsnob with a gradient strength at 24% (13.8 G/cm), resulting in a slice sampling thickness of 0.1 mm. However, the actual slice resolution along the F1 was determined by the incremental frequency of 2000 Hz, which resulted in 0.34 mm. A Topspin command 'xf2' was applied to process the data with a zero-filling, and a line broadening of 0.8 Hz on F2 before the Fourier transform.

(b) Slice projection spectra were taken from the 2D SLS (indicated by the dashed line) corresponding to the cortex and medulla region. The overall spectral profile is nearly analogous to the CPMG spectrum of the individual cortex and medulla tissue. The inserts show a chemical shift expansion of the Cho, GPC, PC, and betaine peaks, displaying the predominant variances (betaine and GPC) between the two regions.

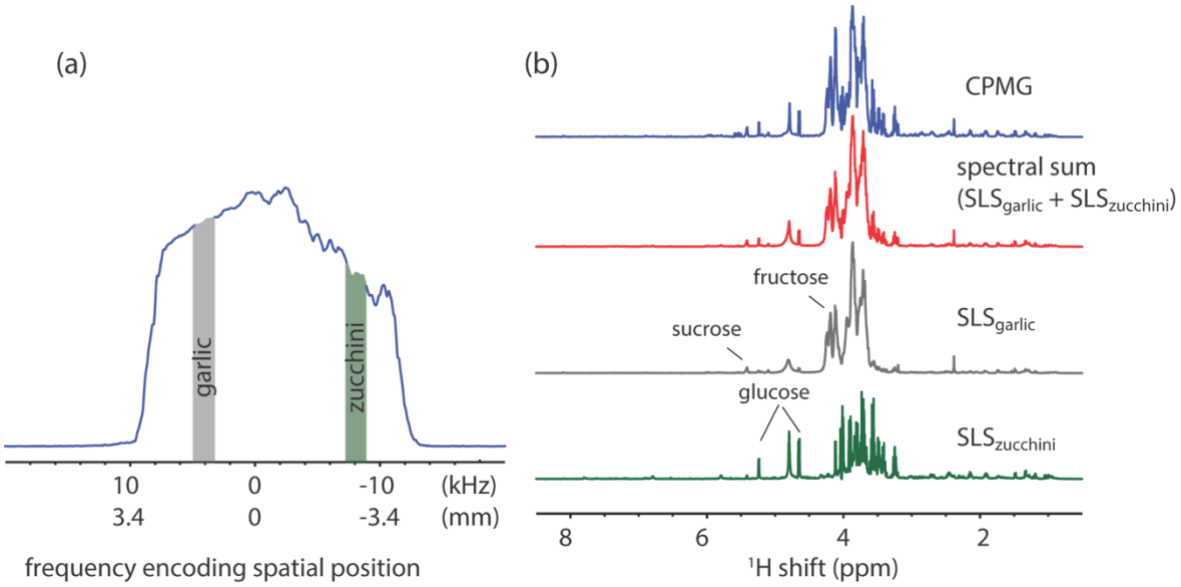

Figure S4. (a) 1D image of a two-layered food phantom (garlic and zucchini) acquired with a 12% gradient strength (6.8 G/cm). (b) Spectral comparison between SLS and CPMG. The red spectrum corresponds to the SLS spectral sum of garlic and zucchini. The blue spectrum was acquired with a CPMG experiment on the whole sample volume. The 1D SLS spectra were acquired with a frequency offset indicated in the 1D image, with a 4 ms ReBurp and a gradient strength at 6% (6.8 G/cm), resulting in 0.5 mm sampling thickness.