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Criteria for Sensitivity Enhancement by Compressed Sensing: Practical application to Anisotropic NAD 2D-NMR Spectroscopy

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Electronic Supplementary Information

Compressed sensing and rapidly decaying sampling schedules

High "randomness" of a sampling schedule is one of the pre-requisites for an effective CS reconstruction. "Random" sampling schedules generated with rapid decay of sampling density are in fact similar to truncated conventional sampling schemes. It was already shown by Stern et al.,[1] that application of CS algorithm (l_p-norm minimization in this case) for signal "extrapolation" leads to false peak splitting.

Fig. S1 shows typical peak distortions observed for rapidly decaying sampling schedules. All CS algorithms used so far in NMR (including the one applied in this study) start from vector **S** obtained by the direct FT of the NUS signal (green line in **Fig. S1**) and the CS reconstructed spectrum is calculated from **Eq. 9** (See article). The effect of the sampling decay on the shape of peaks obtained by direct FT is exactly the same as the effect of weighting function [2,3]. Hence, rapid decay causes peak broadening and such broaden peak is used as a starting point for the reconstruction (green line in **Fig. S1a**). As described in ref. 1 and depicted in **Fig. S1a** (blue line), the application of sparsity-enforcing reconstruction, such as CS, produces false peak splitting, as the broad peak is approximated by sparser artificial multiplet. For instance, **Fig. S1a** shows that CS reconstruction of NUS FID sampled with rapidly decaying schedules (T_S = 0.01 s) modifies the peak height and produces artificial "triplet" structure. When sampling density decay

is slower, the sampling is more random and the restricted isometry constants are lower, which guarantees high-fidelity reconstruction. For instance, **Fig. S1b** shows that for T_S = 0.15 s, the starting vector **S** exhibits correct peak width but differ from the oracle solution in peak height and by noise-like artefacts. However, these differences vanish in the CS-reconstructed spectrum, which accurately reproduces the oracle spectrum.

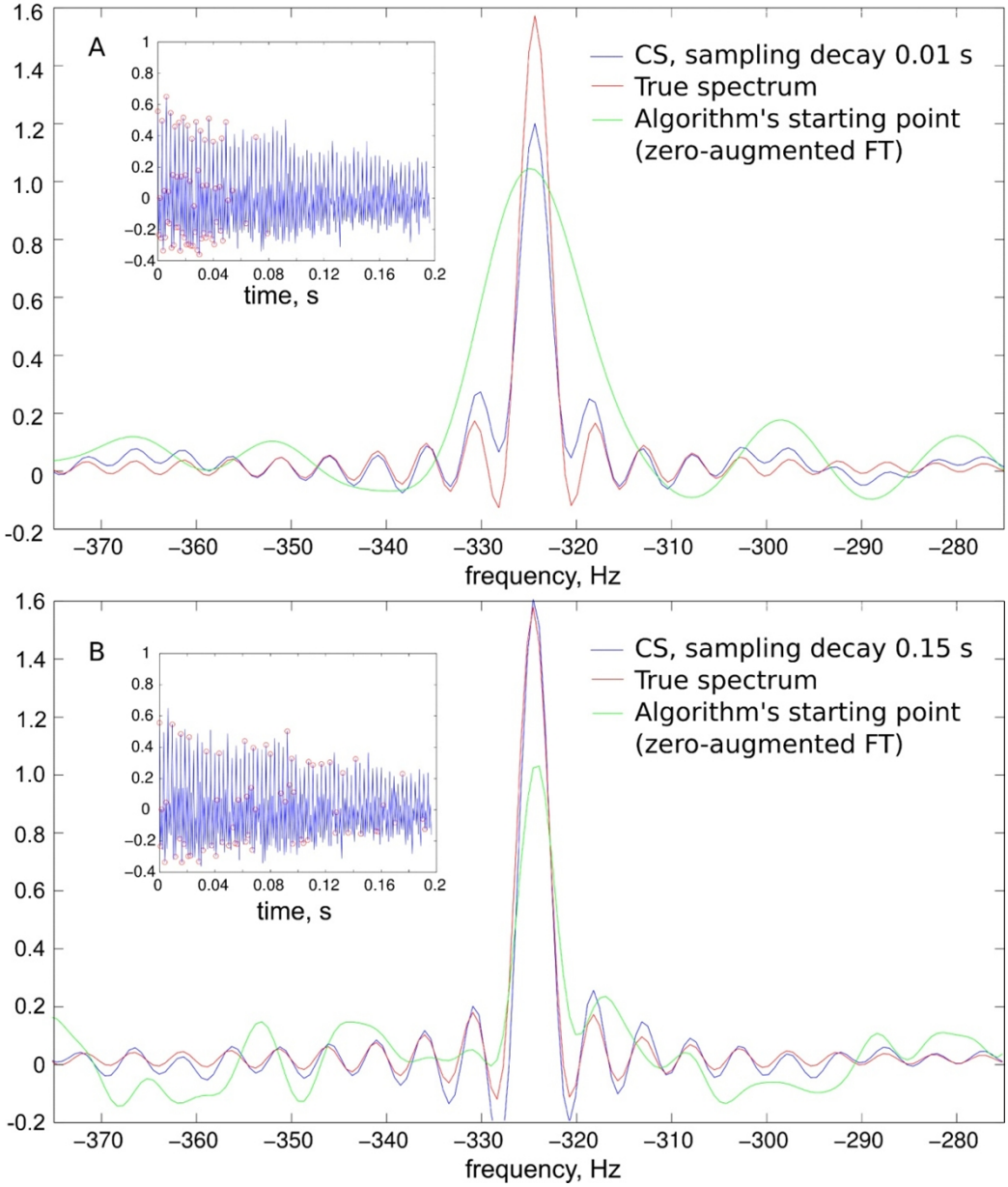

Fig. S1 Line shape for different sampling schedules and processing procedures of the simulated FID identical to shown in **Figure 5** of the main text, but without noise. The signal was zerofilled to 2048 points (in case of CS after the reconstruction). The spectra displayed in this figure are expanded near the S2 peak. Red line shows the oracle spectrum obtained by FT of noiseless US FID with 256 sampled points, blue line shows the CS reconstruction of NUS FID with 64 points and green line shows the spectrum obtained by FT of NUS FID, which is a starting point of CS algorithm. The NUS FIDs are generated with T_S = 0.01 s in A and 0.15 s in B. Insets illustrate the used sampling schedules.

References

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