Supplemental Information: Exploring Signal-to-noise Ratio and Sensitivity in Non-Uniformly Sampled Multi-Dimensional NMR Spectra

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Supplementary Table 1: Comparison of the accuracy of peak heights between different sampling procedures and hmsIST reconstruction. The same spectrum as in Fig. 1 was used but simulated with 100 sets of random noise using different seed numbers. As can be seen the standard deviation for the peak height does not decrease with time-equivalent sparse sampling.

	Peak #1	Peak #2	Peak #3	Peak #4
No noise	288	144	72	36
100% US	287.9 ± 6.9	144.1 ± 6.4	71.8 ± 6.1	35.5 ± 6.2
25% NUS	287.0 ± 5.0	143.2 ± 5.9	67.1 ± 5.7	31.3 ± 6.6
10% NUS	291.6 ± 6.8	138.7 ± 6.0	64.9 ± 6.4	22.9 ± 7.0





Supplemental Figure S1: Histogram of the noise distribution in US and NUS spectra. The histogram provides values for standard deviation (rms) and normalized kurtosis. As a kurtosis of a Gaussian distribution is 3.0 we have subtracted a number of 3.0 to obtain a normalized kurtosis and see the deviation from a Gaussian distribution. Kurtosis values > 0 indicate a narrower, sharper distribution. The data are obtained on the 2k complex data set in figure 1b-d.



Supplemental Figure S2: Comparison of the 1D slices from panels Fig. 2E (64 ¹⁵N x 128 ¹H points, NS = 4, 500 MHz, RT probe) and 2F (6.25% sampled from 64 ¹⁵N x 128 ¹H points, NS = 64, 500 MHz, RT probe) with the corresponding slice from a high resolution uniformly sampled spectrum (64 ¹⁵N x 1200 ¹H points at 900 MHz and cryoprobe). Thus, the peaks labeled with "*" in Fig. 2F correspond to real peaks.