Electronic Supplementary Material for PCCP

Isotropic Chemical Shifts in Magic-Angle Spinning NMR Spectra of Proteins

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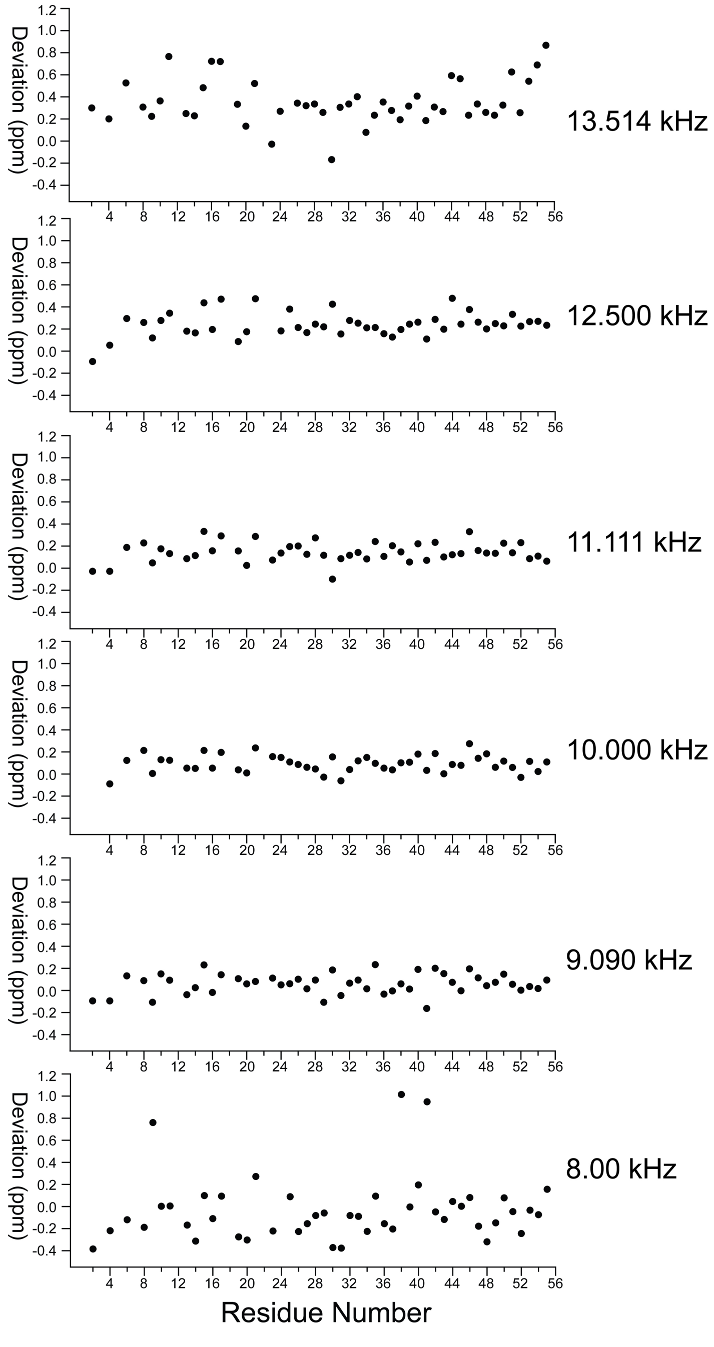
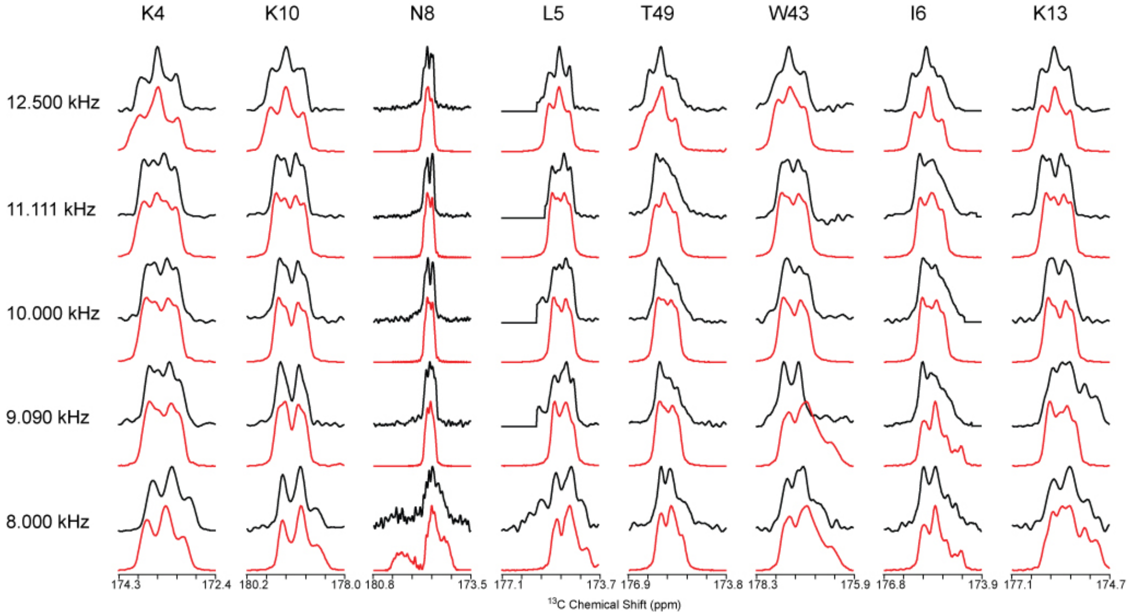
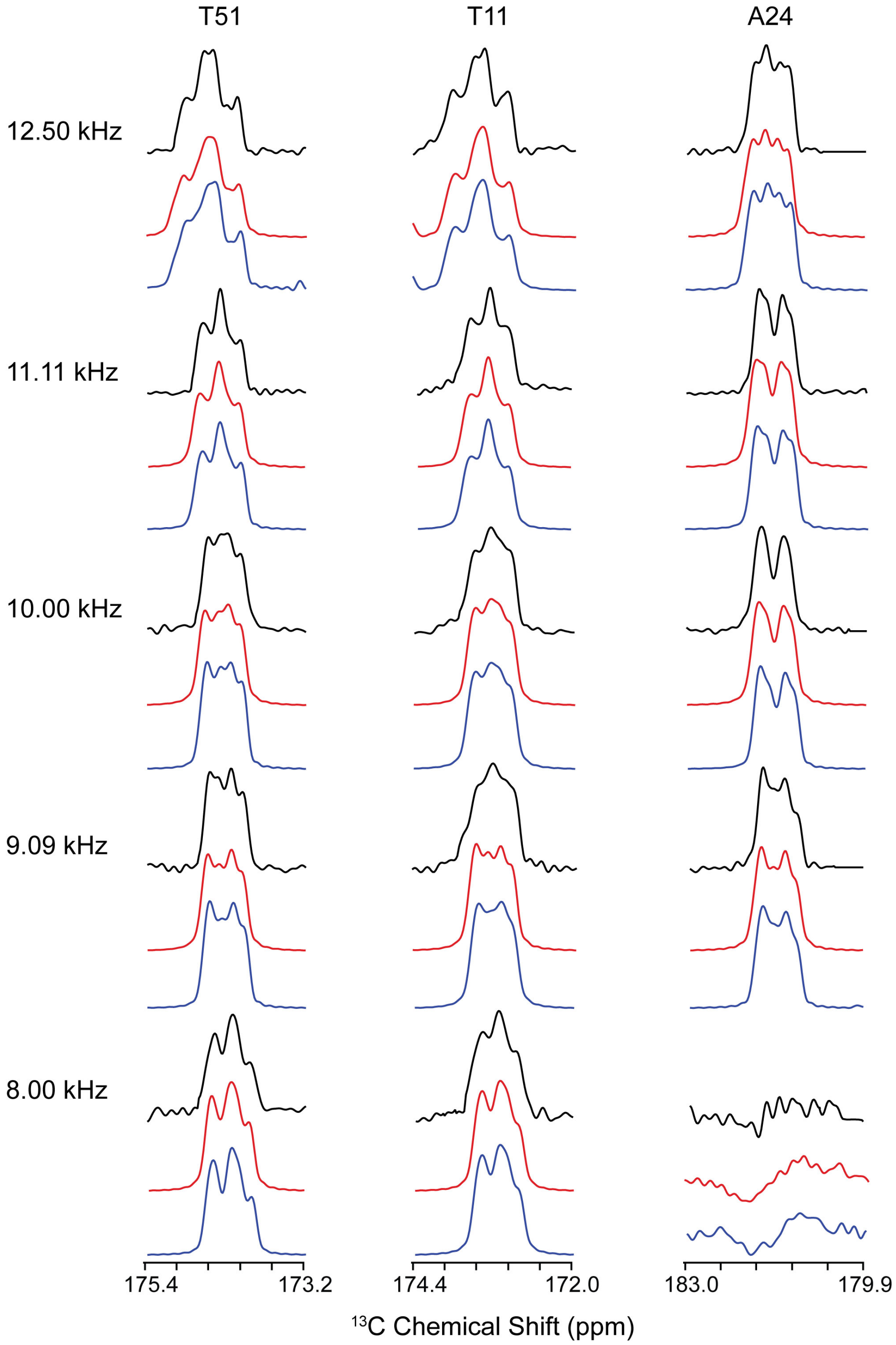
Supporting Information



Supporting Figure 1. Residue-specific deviations of measured $^{13}C'$ isotropic chemical shifts in GB1. The deviation is defined as the difference of observed peak position measured in the U-^{13}C-labeled sample from the position measured in the sample prepared from 1,3-^{13}C-glycerol. Experiments were performed at 500 MHz ^{1}H frequency, with further details included in the main text.



Supporting Figure 2. Exemplary experimental lineshapes (black) and best fit simulations (red) for carbonyl signals in U-^{13}C,^{15}N-labeled GB1. Experiments were performed at 500 MHz ^{1}H frequency.



Supporting Figure 3. Examples of experimental lineshapes (black) and best fit 2-spin simulations (red), and best fit 4-spin simulations (blue). Differences between 2-spin and 4-spin simulations within the experimental relaxation and SNR are minimal.