Supporting Information

Application of geometric approximation to the CPMG experiment: two- and three-site exchange

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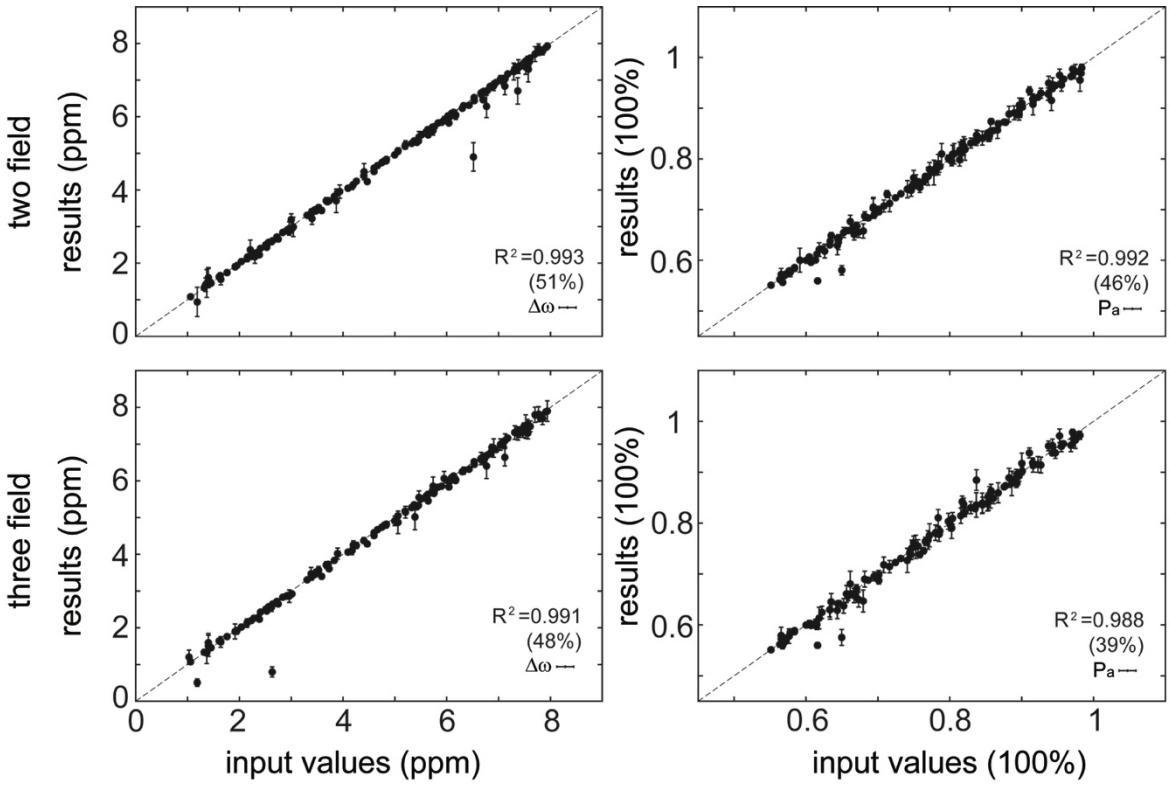
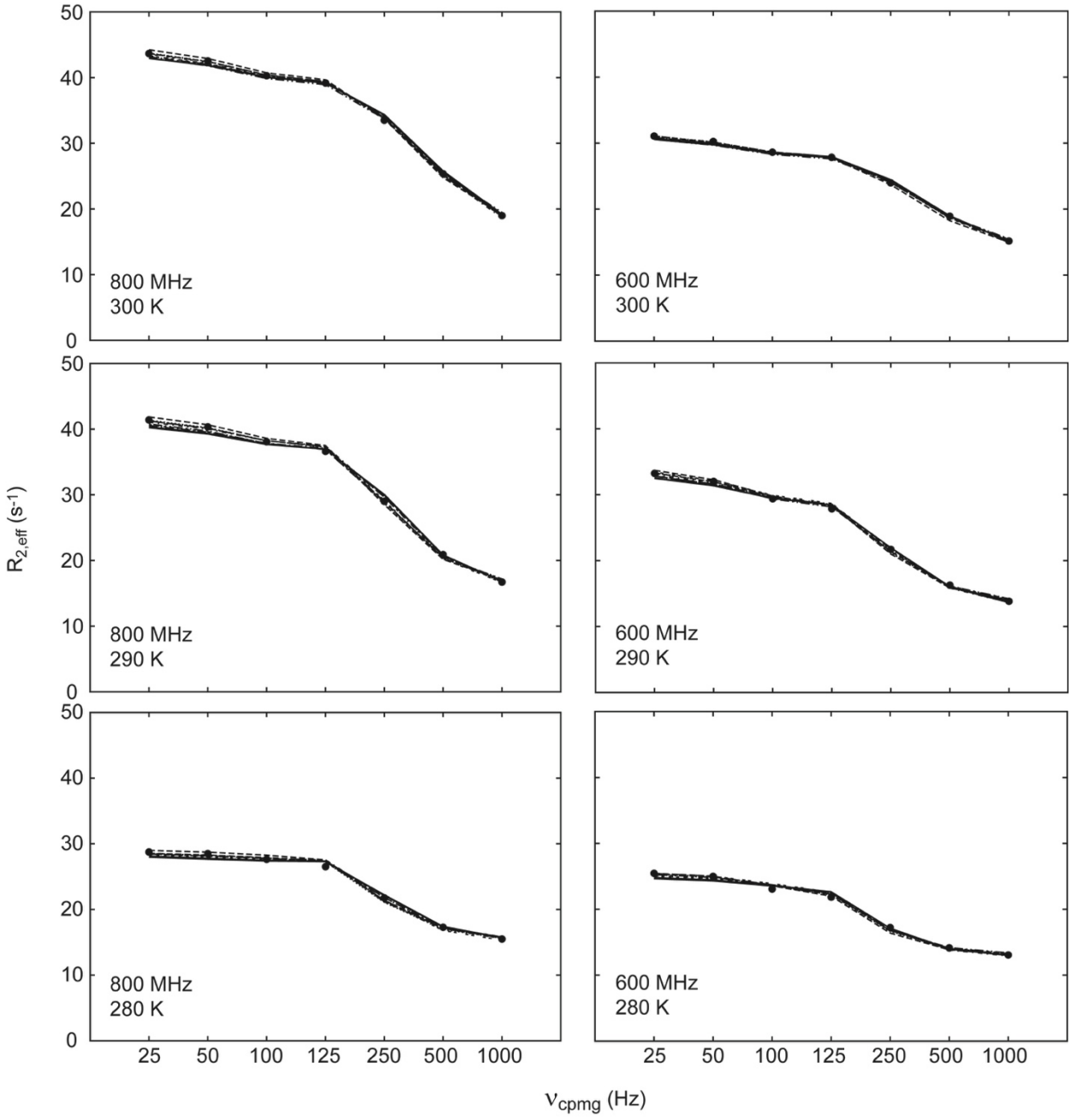


Supporting figure 1. Fitting the simulated relaxation data of constant-time CPMG experiments (40 ms) in the 2-site exchange model at two (14.1T, and 18.8T) or three (14.1T, 16.5T, and 18.8T) magnetic fields using geometric approximation. The 300 data sets of different CPMG frequencies (νCPMG = 25, 50, 100, 125, 250, 500, 1000 Hz) were simulated using Bloch-McConnell equation with random dynamic parameters. The fit results are plotted against the input values, and those with large standard deviations (S.D. of $\Delta\omega$ > 0.4 ppm, and S.D. of p_a > 2.5%) during Monte Carlo sampling are not shown. The coefficient of determination (R^2) is calculated for each case. The numbers in the parentheses are the percentages of the data remained after filtering out the results with large standard deviations.



Supporting figure 2. Fitting the simulated relaxation data of constant-time CPMG experiments (40 ms) in the 3-site exchange model with temperature variation (280 K, 290 K, and 300 K) and two magnetic fields (14.1 T, and 18.8 T) using geometric approximation and the 2-site exchange model. The data set of different CPMG frequencies (νCPMG = 25, 50, 100, 125, 250, 500, 1000 Hz) was simulated using the modified Bloch-McConnell equation with given dynamic parameters, which are plotted as points. The 10 best fit out of 100 fit results are plotted as lines after Monte Carlo sampling.