Supplementary Information

Asynchronous through-bond homonuclear isotropic mixing: Application to carbon-carbon transfer in perdeuterated proteins under MAS

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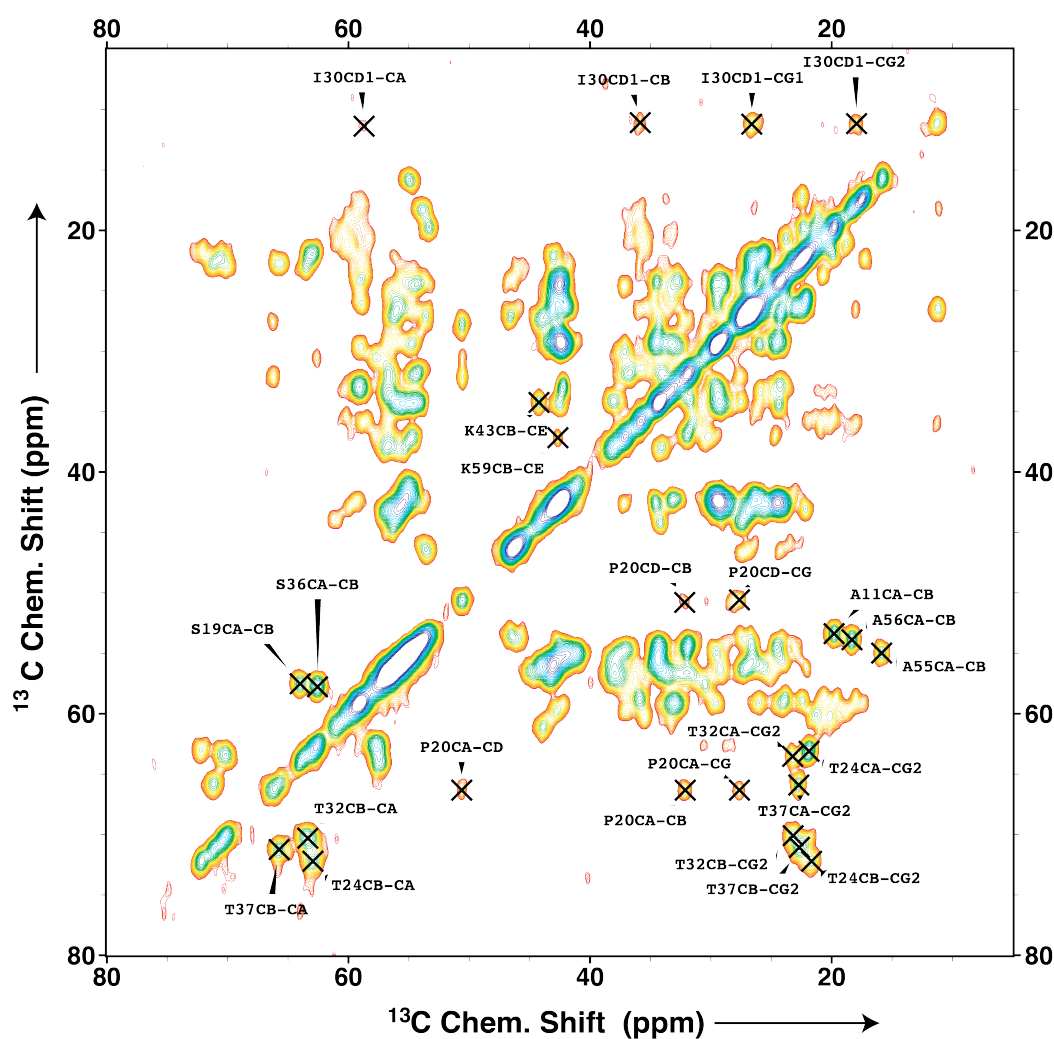
Fig. S1. 2D ^{13}C-^{13}C correlation experiment using the hard-pulse MOCCA sequence. A partial assignment, indicating a selection of resolved peaks used for quantitative analyses is shown here.
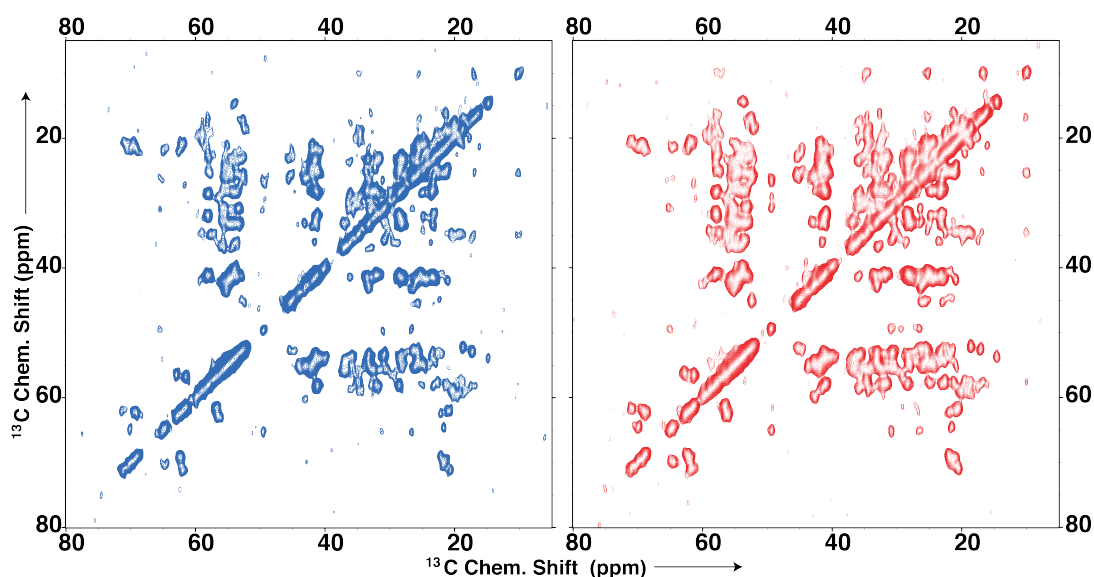
Fig. S2. 2D spectral examples representing the performance of MOCCA with longer CP contact time (of 1.8 ms) with a delay $\Delta = 60$ μs and $\Delta = 100$ μs between the pulses, using total mixing times of 33 ms and 53 ms on the left and the right, respectively. Each 2D spectrum was recorded in 10 hours.
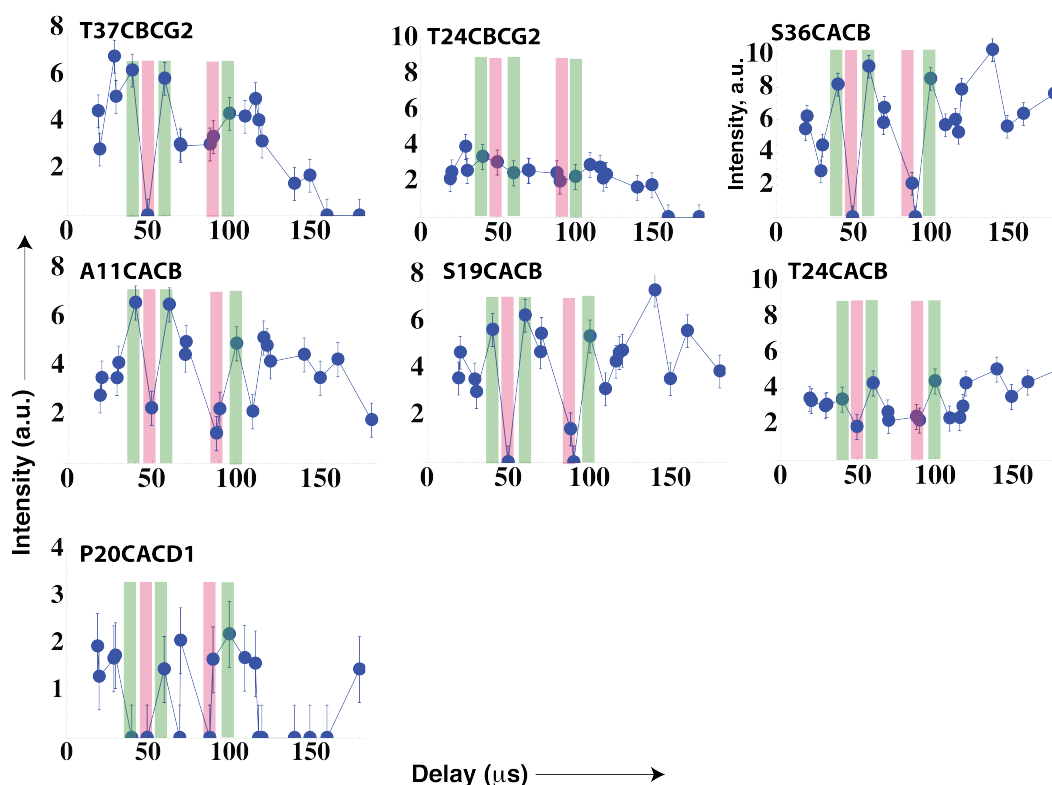

Fig. S3. Further examples for experimental optimization of the hard-pulse MOCCA, adding to peaks shown in Main Text Figure 2. The different cross-peak intensities upon large-scale variation of the delay Δ are depicted. The total mixing time in all experiments was set to 15 ms. Minimum and maximum transfer efficiency transfer regions are shown in purple and green colors, respectively.
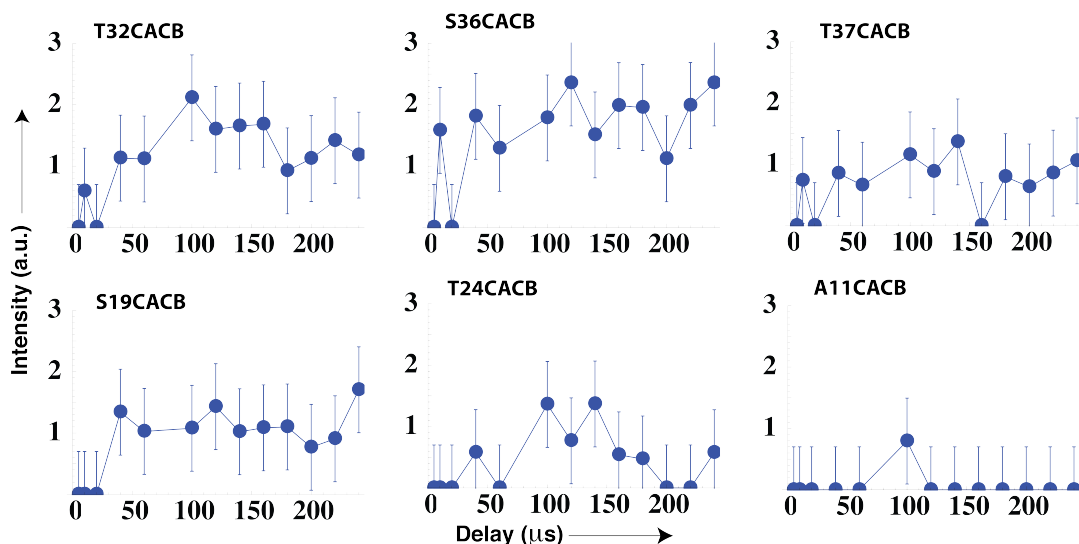
Fig. S4. Experimental optimization of the delay Δ for soft-pulse MOCCA. Again, the different cross-peak intensities upon large-scale variation of the delay Δ are depicted. The total mixing time in all experiments was set to 15 ms.
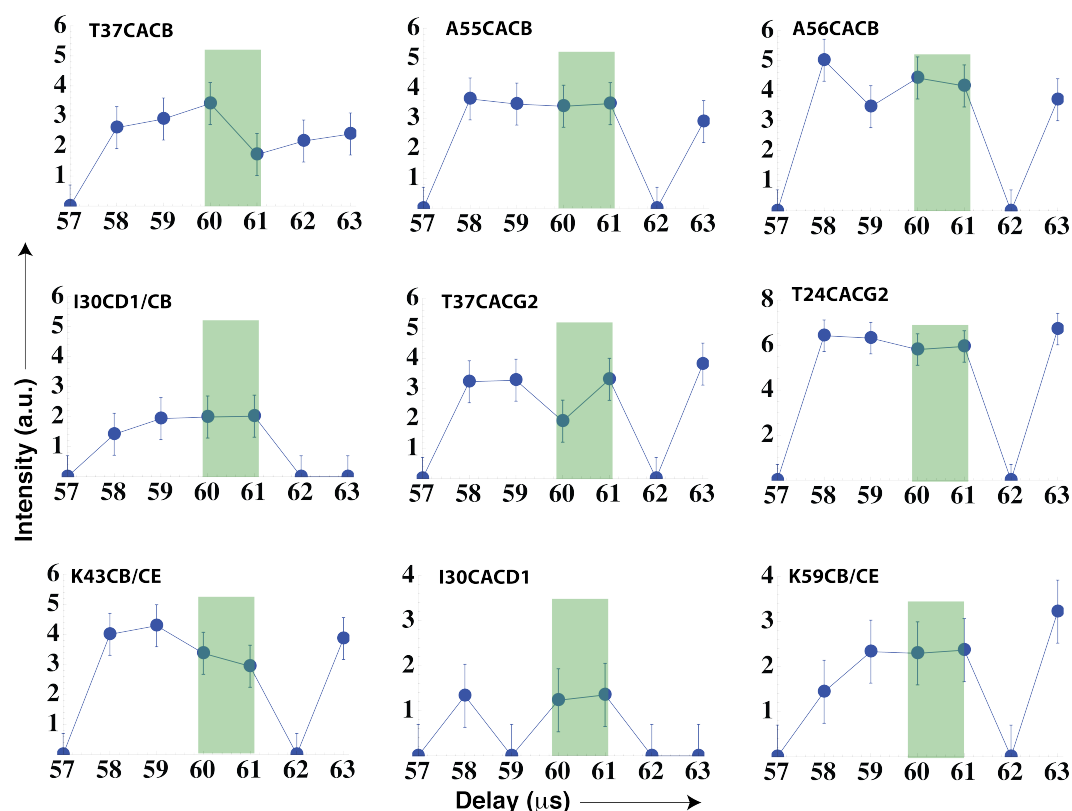

Fig. S5. Experimental optimization of the delay for the MOCCA hard pulse scheme. Here, the variation of cross-peak intensity as a function of the delay Δ is shown for variation with fine steps around the global maximum. The total mixing time in all experiments was set to 15 ms.
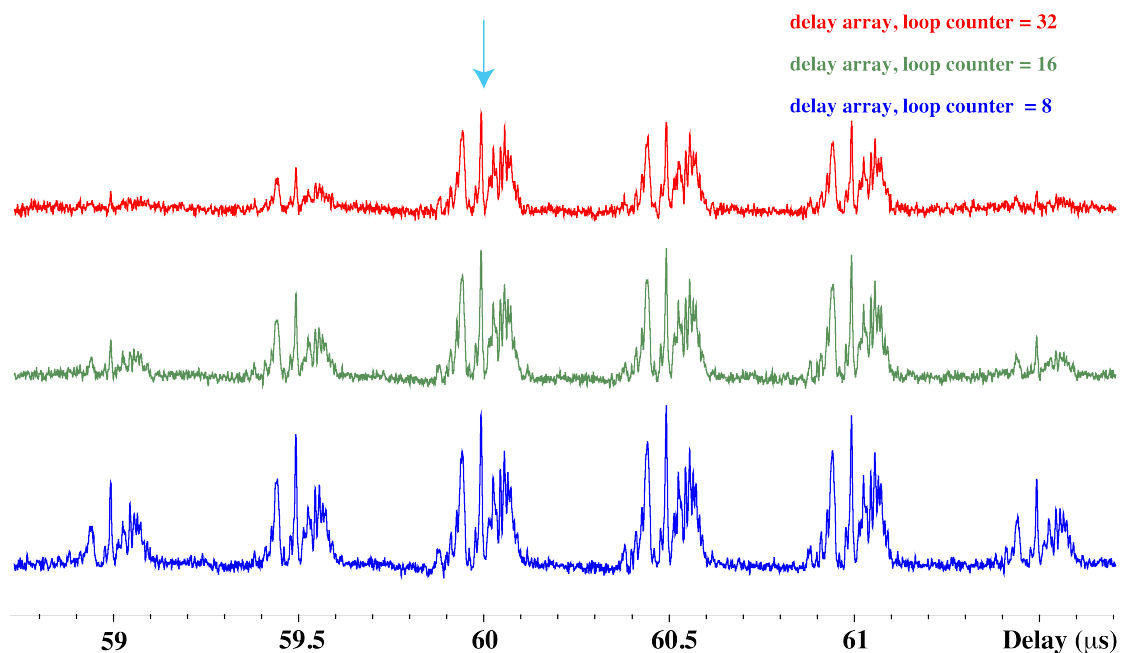
Fig. S6. Experimental optimization of the delay for the MOCCA hard pulse in a 1D mode, using three different loop counters. Here, the peak intensity reaches minimum values every ¼ τ_r. The chosen numbers of loop counters (one loop contains 16 pulses with different phases) correspond to 9 ms (blue), 18 ms (green) and 36 ms (red). The plot represents an excerpt of the optimization for delay values around the global optimum (here 60 μs).