Supplementary information:

Configurational Entropy Components and Their Contribution to Biomolecular Complex Formation

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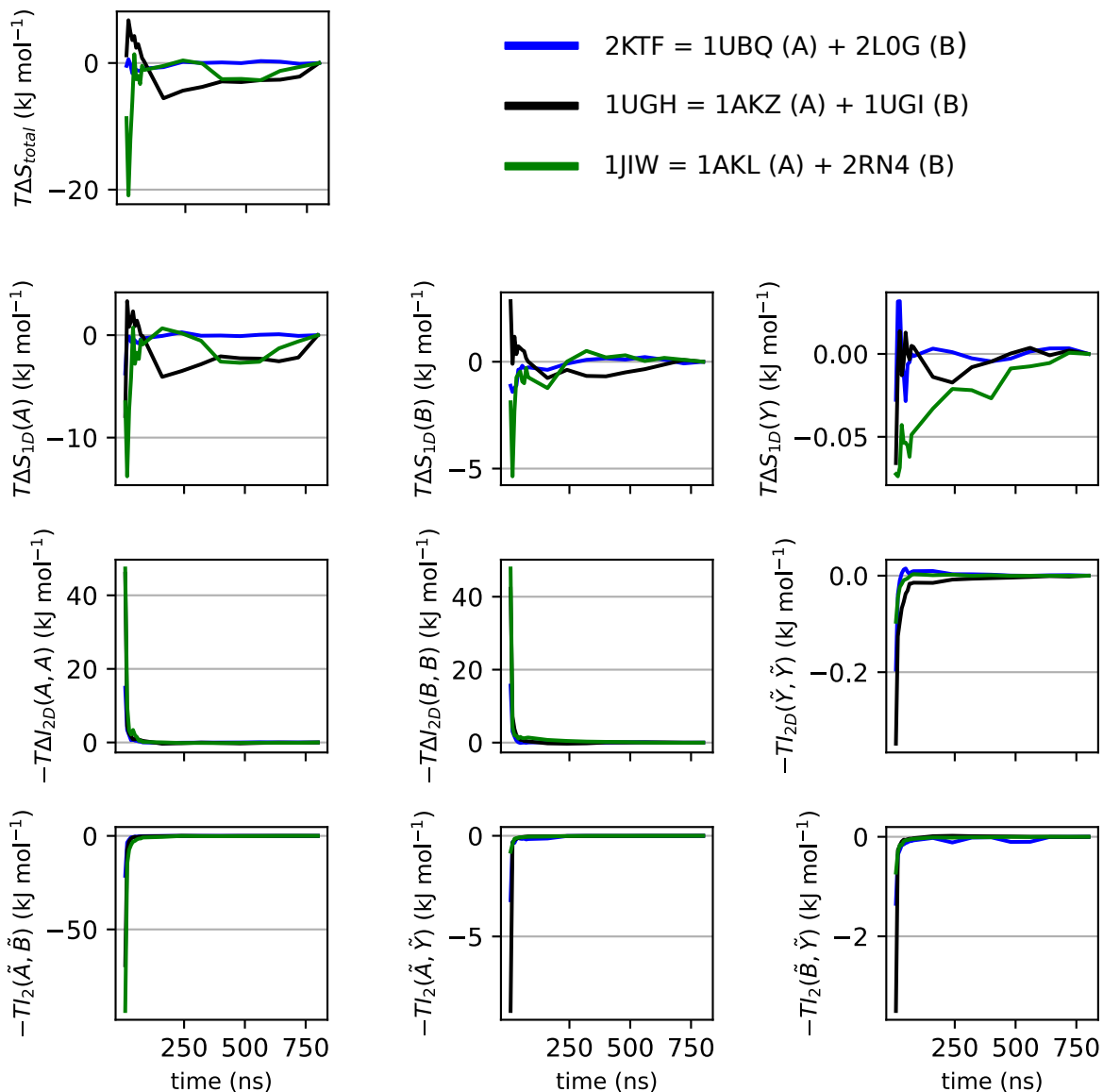
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Figure 1: Convergence analysis of three representative complexes from shuffled trajectories. The analysis here is the same as in Figure 2 of the main article, but with the frames in the original trajectories shuffled randomly. By removing time ordering, this analysis captures convergence as a function of ensemble size (frames) as opposed to simulation time. Because the convergence with ensemble size is considerably more rapid, the first 80 ns have been fine-grained to 8 ns spacing of data points. The resolution of the trajectories is 1 ps.