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Supplemental Information

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Supporting Material

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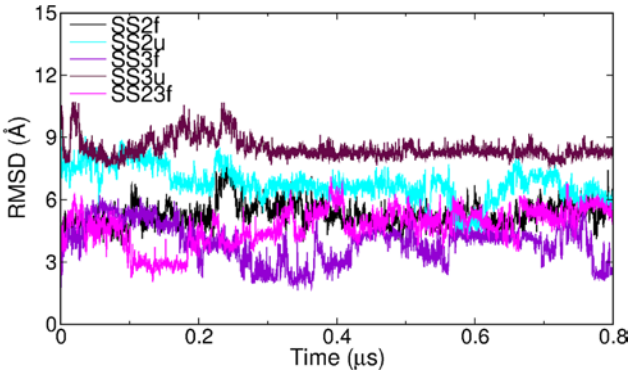

Fig. S1 RMSDs measured for Cα atoms for structures of MCoTI-II in different conditions; RMSD values were determined all relative to the native structure.

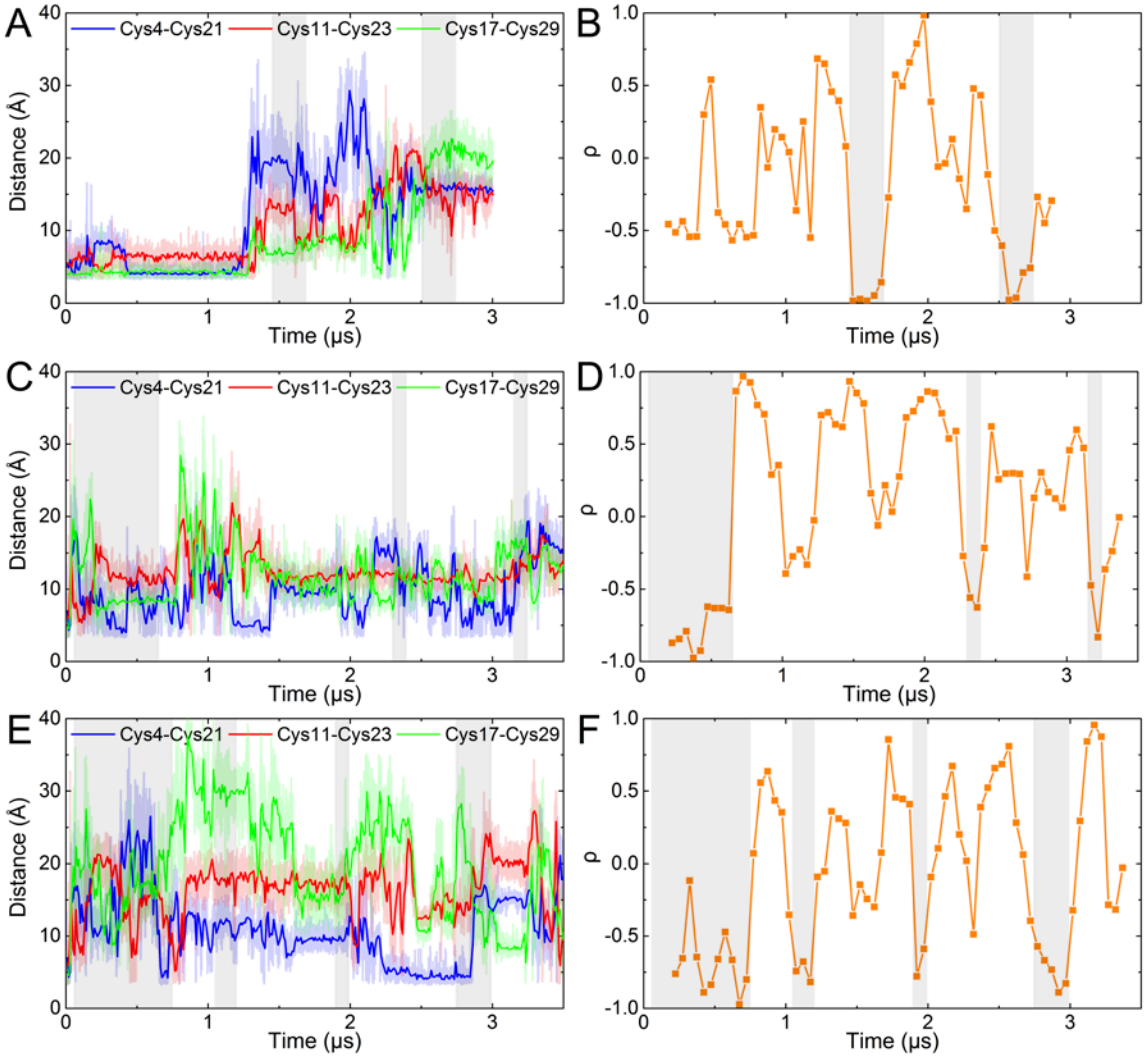

Fig. S2 Sulfur-sulfur distances and correlations monitored in simulations of different conditions. A. Sulfur-sulfur distances monitored in simulation SS0f(b). Average distances taken over 0.01 μs windows are shown as bold traces; light traces show raw distance data. Grey shading highlights the time when Cys11-Cys23 and Cys17-Cys29 distances are anti-correlated. B. Pearson correlation coefficient between Cys11-Cys23 and Cys17-Cys29 distances in simulation SS0f(b) from panel A. A gliding window of size 0.3 μs and step 0.05 μs is applied to monitor correlation as a function of time. The same grey shading as in panel A cover the time when large negative correlation coefficients are present. C. and D. Same as A. and B. for simulation SS0u(b). E. and F. Same as A. and B. for simulation SS0u(c).

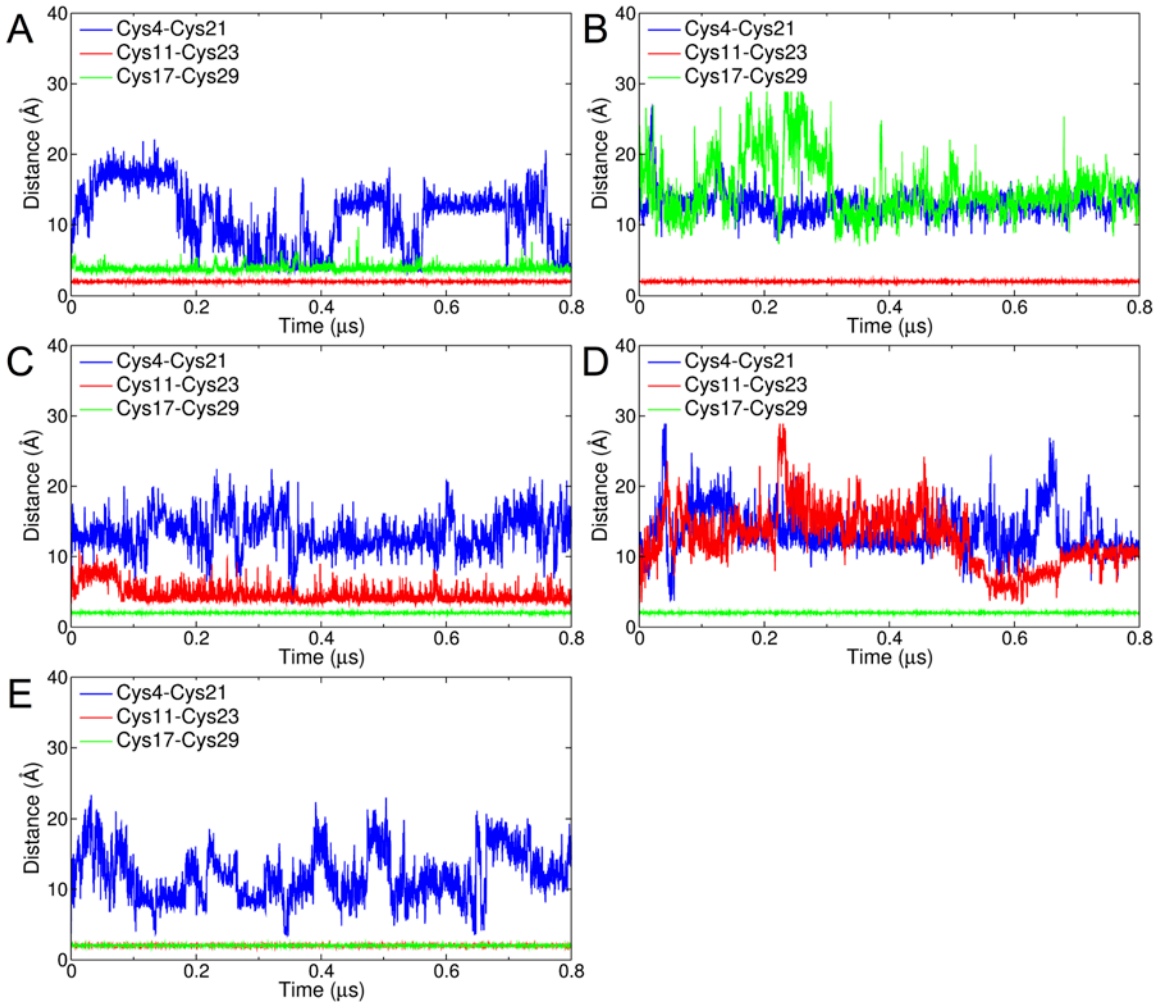

Fig. S3 Sulfur-sulfur distances monitored in simulations of different conditions: A. SS2f B. SS2u C. SS3f D. SS3u and E. SS23f.

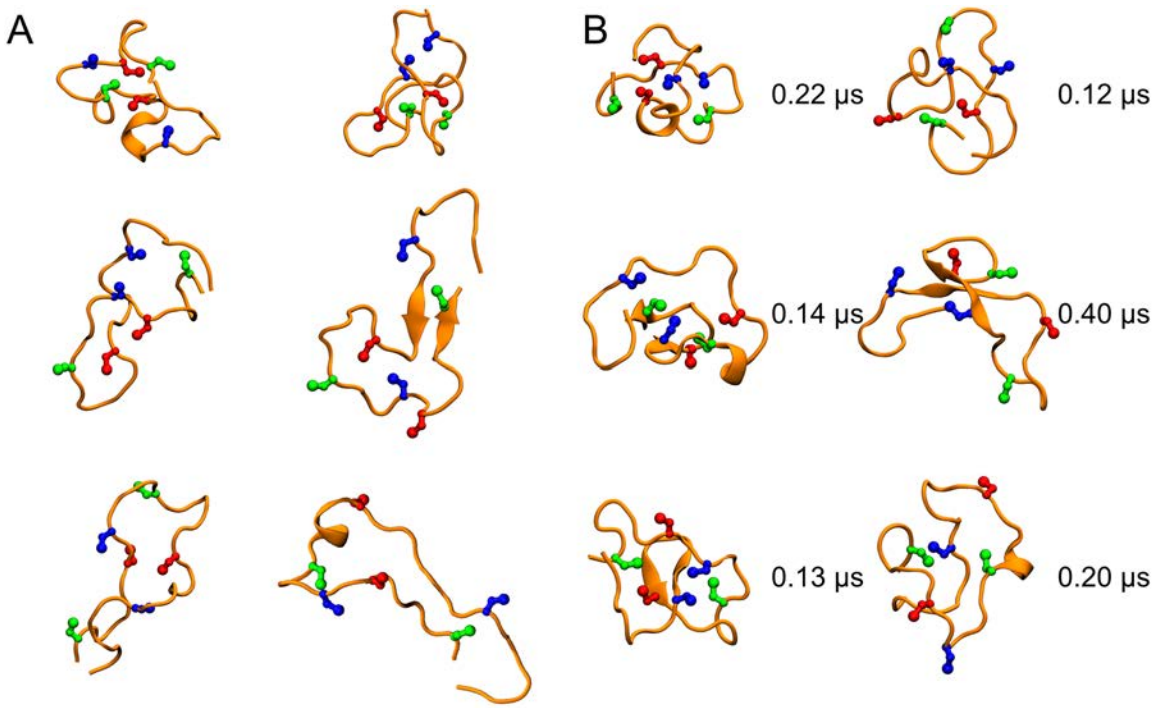

Fig. S4 A sampling of both anti-correlated and correlated structures in SS0f(a, b) and SS0u(a, b, c) . A. Randomly selected structures from highly mobile states right after the initial unfolding transitions in simulations, where distance 11-23 and distance 17-29 is anti-correlated. B. Representative structures of peptide trapped in less native-like microstates, labeled on the right with approximate lifetime for each microstate. The structures in these microstates were stabilized by secondary structures (alpha helix/beta sheet) and were more compact and less mobile compared with structures in panel A. The anti-correlation between distance 11-23 and distance 17-29 disappears in these microstates.