

Supemental data

Role of the sulfur to α -carbon thioether bridges in thurincin H

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Figure S1. Heat capacity curves of Thurnincin H calculated the consecutive sections of the MREMD simulation without harmonic potentials imposed on the thioether bonds. The 50,000,000 step range (with 25,000 \times 64 snapshots total) was divided into 8 slices (with 200,000 snapshots each) and the respective heat-capacity curves are colored red, orange, yellow, green, cyan, blue, purple, and black for slices 1 – 8, respectively.

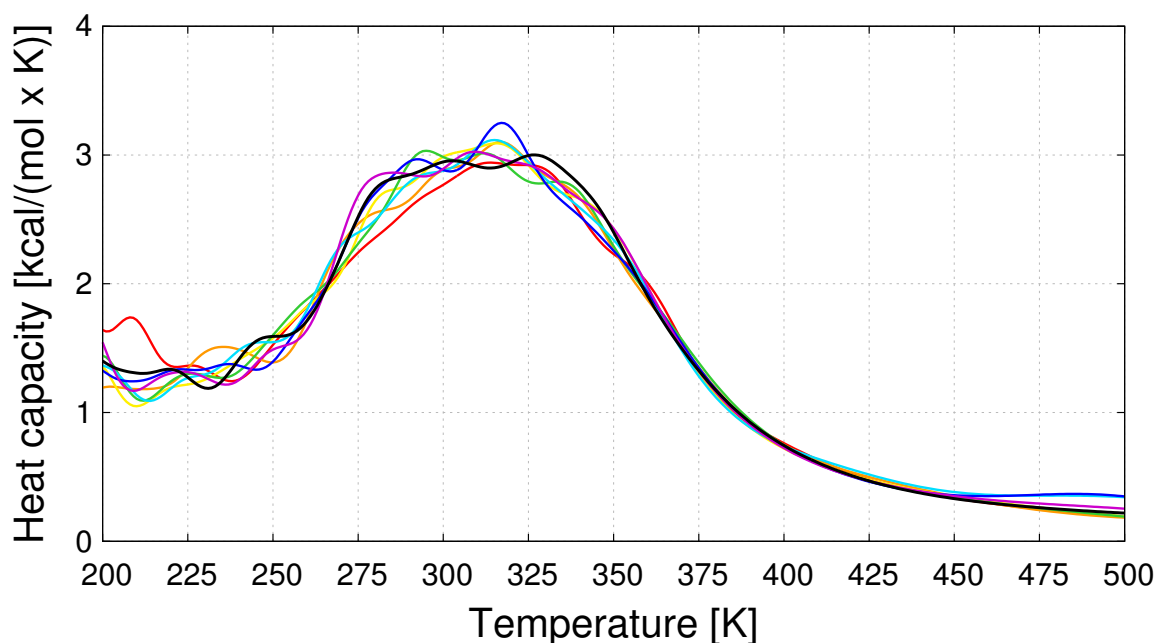


Figure S1

Figure S2. Plots of the fractions of the folded structures (in the temperature from 250 K to 375 K) obtained in the series of unfolding MREMD simulations with the thioether bonds gradually turned off. Each panel corresponds to a given order of switching off the thioether bridges and different graph colors correspond to the the simulation with all 4 bridges (purple), 3 bridges (red), 2 bridges (orange), and 1 bridge (green). The bridged residues are shown in the graphs and color-coded according to the number of bridges.

