

Supplemental Information

Structural and Dynamic Evolution of the Amphipathic N-terminus Diversify Enzyme Thermostability in the Glycoside Hydrolase Family 12

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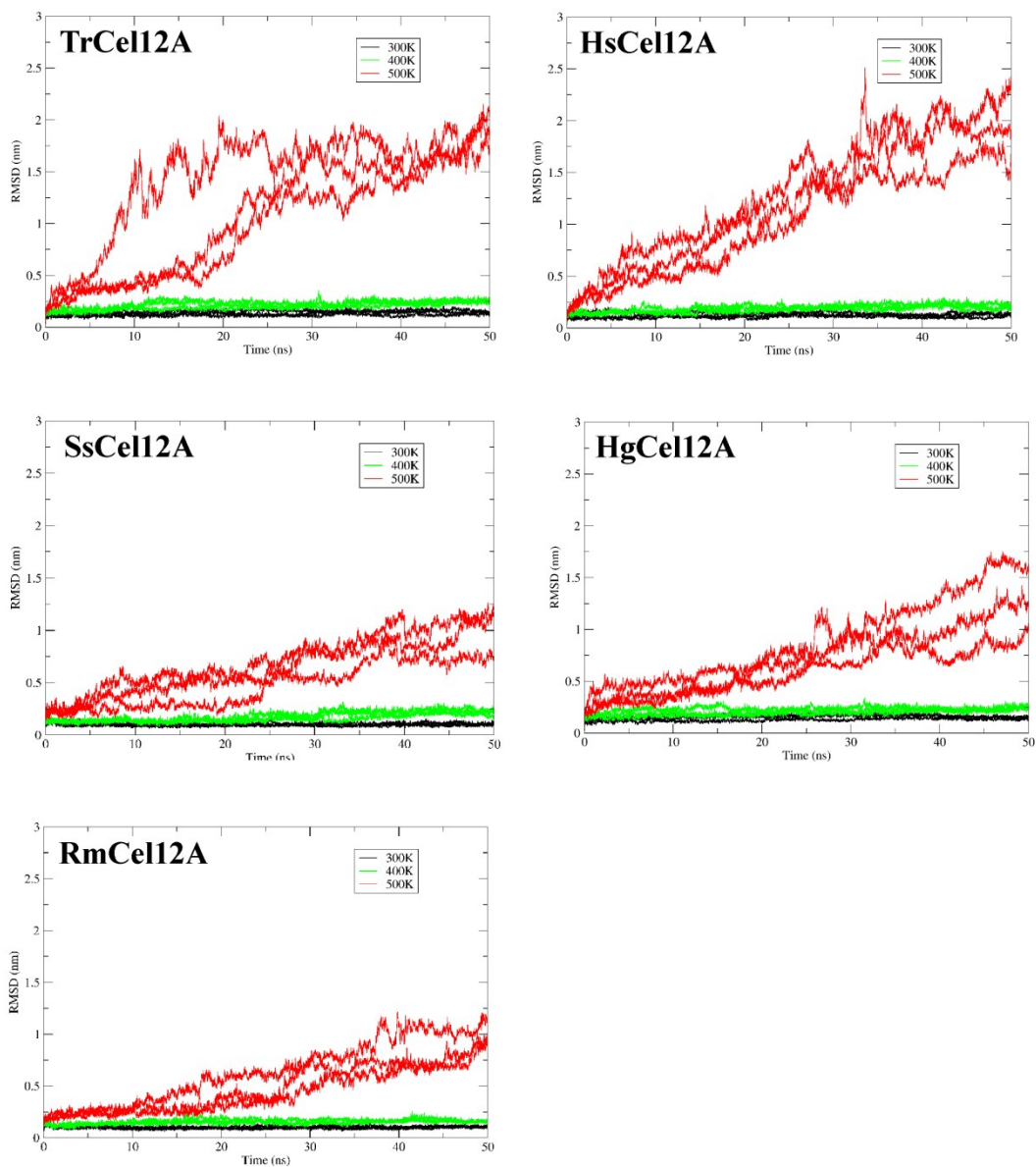


Figure S1. Time evolution of the backbone RMSD for GH12 *enzymes*. The calculated data obtained from the simulations at 300, 400, and 500K with three replicas are shown in *black*, *green* and *red*, respectively.

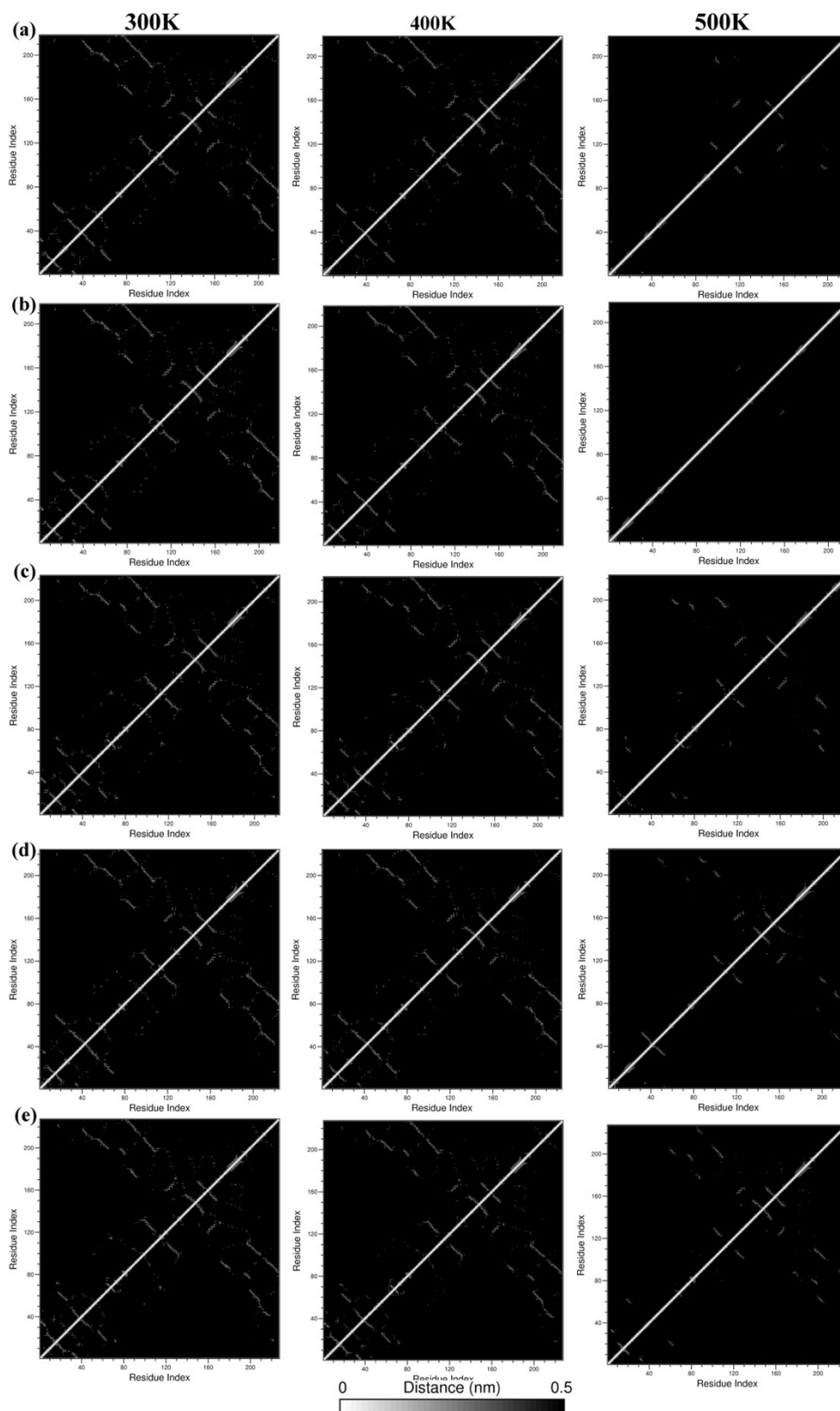


Figure S2. The smallest distance matrices between residue pairs at 300, 400 and 500 K. A contact is defined if the distance is less than 0.5 nm. (a-e) indicate TrCel12A, HsCel12A, SsCel12A, HgCel12A and RmCel12A.

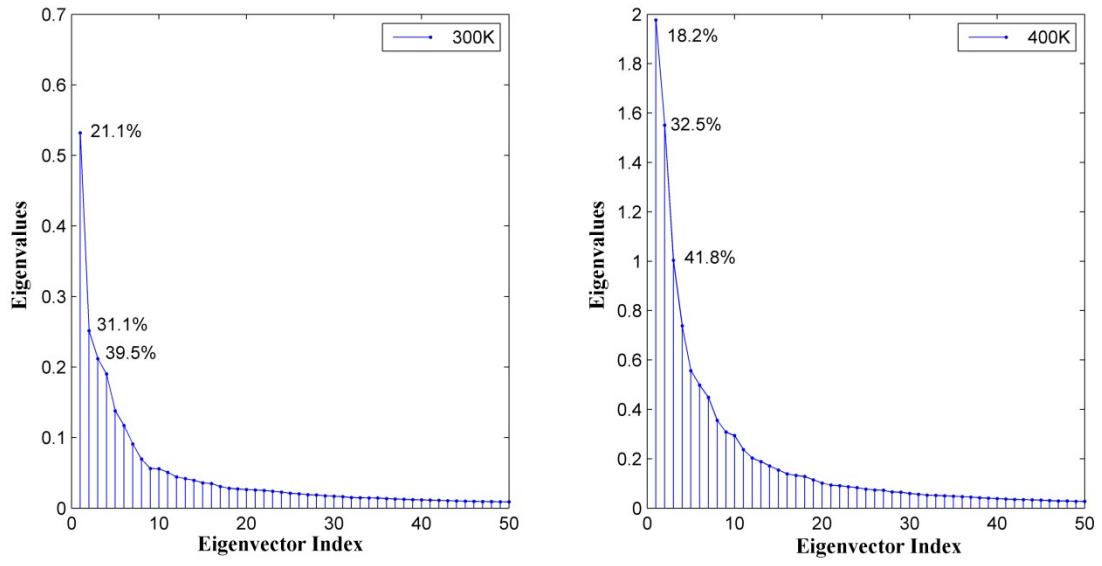


Figure S3. The eigenvalues against its eigenvector index. The proportion of variance of the first three eigenvectors were labeled.

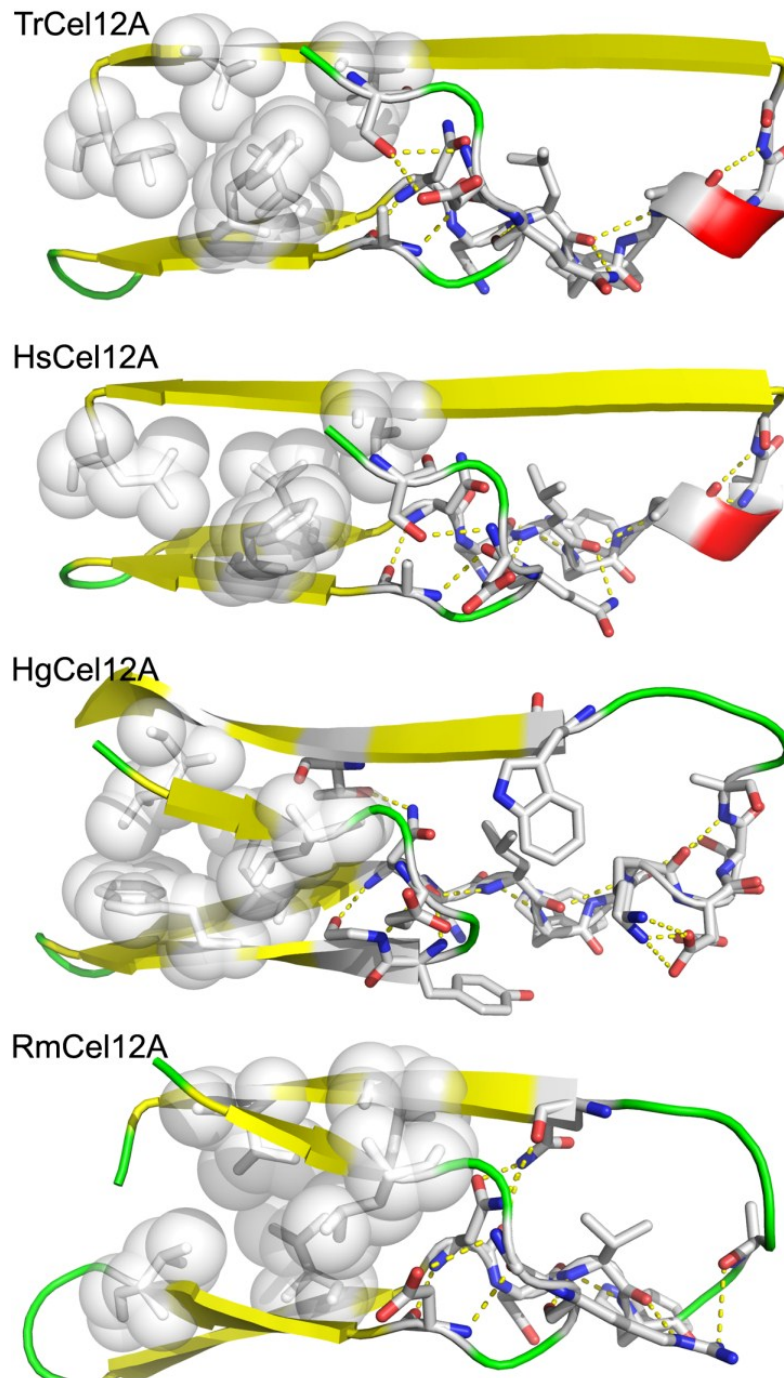


Figure S4. The amphipathic pattern of internal interactions within the N-terminus. The residues that participate in hydrophobic packing core and the hydrogen bonding network were shown in sphere and lines models, respectively.