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Research article

Globular bundles and entangled network of proteins (CorA) by a coarse-grained Monte Carlo simulation

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Supplementary material

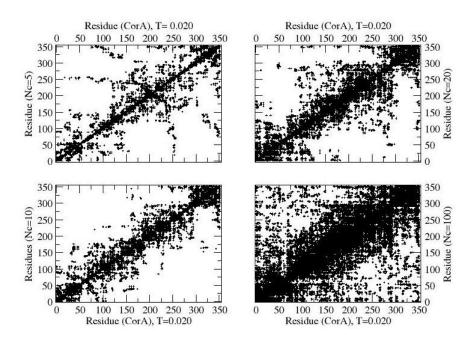


Figure S1. Contact map of residues around each of CorA (${}^{1}M {}^{2}E \dots {}^{351}L$) residues in a simulation box with the number of protein chains Nc = 5, 10, 20, and 100 at a low temperature (T = 0.020).

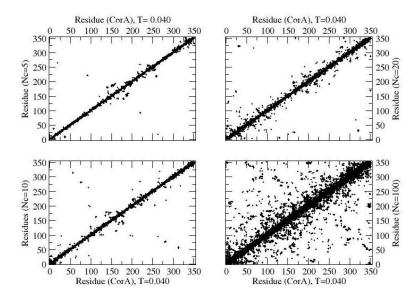


Figure S2. Contact map of residues around each of CorA (${}^{1}M {}^{2}E \dots {}^{351}L$) residues in a simulation box with the number of protein chains Nc = 5, 10, 20, and 100 at a high temperature (T = 0.040).

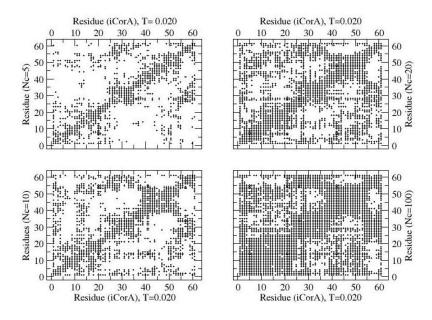


Figure S3. Contact map of residues around each of iCorA residues (${}^{1}M {}^{2}V \dots {}^{61}L$, corresponding sequence in CorA ${}^{291}M {}^{293}V \dots {}^{351}L$) in a simulation box with the number of protein chains Nc = 5, 10, 20, and 100 at a low temperature (T = 0.020).

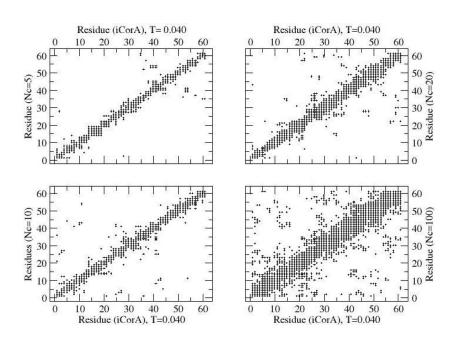


Figure S4. Contact map of residues around each of iCorA residues (¹M ²V ... ⁶¹L, corresponding sequence in CorA ²⁹¹M ²⁹³V ... ³⁵¹L) in a simulation box with the number of protein chains Nc = 5, 10, 20, and 100 at a high temperature (T = 0.040).

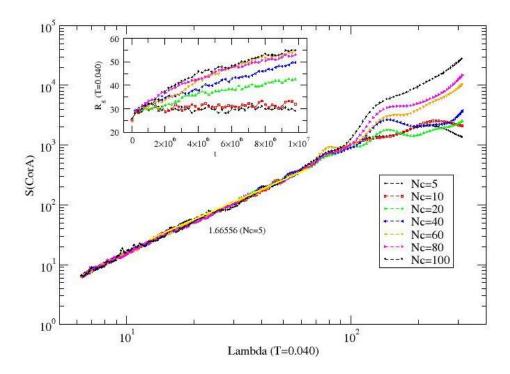


Figure S5. Structure factor S(q) versus the wave length (Lambda λ) at temperature T = 0.040 with a wide range of the number Nc (5–100) of CorA proteins in simulation box. The inset shows the variation of the radius of gyration of proteins with the number Nc (5–100) of CorA proteins in simulation box.



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