

Supplementary Material

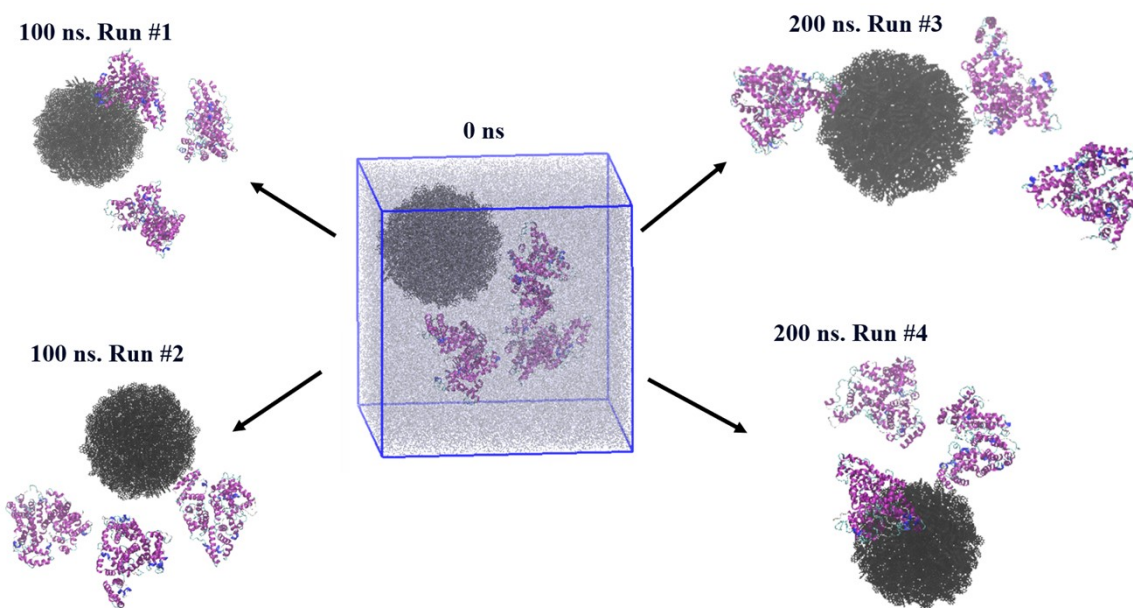


Figure S1. Visualized simulation boxes at the beginning and the end of the MD simulations. The water molecules and ions are not shown for clarity at the end of the simulations. Coloring methods: black: 9-nm CB-NP model; ice-blue: water; the secondary structure of the BSA protein: blue and violet: helices, white and cyan: unstructured bend and turn.

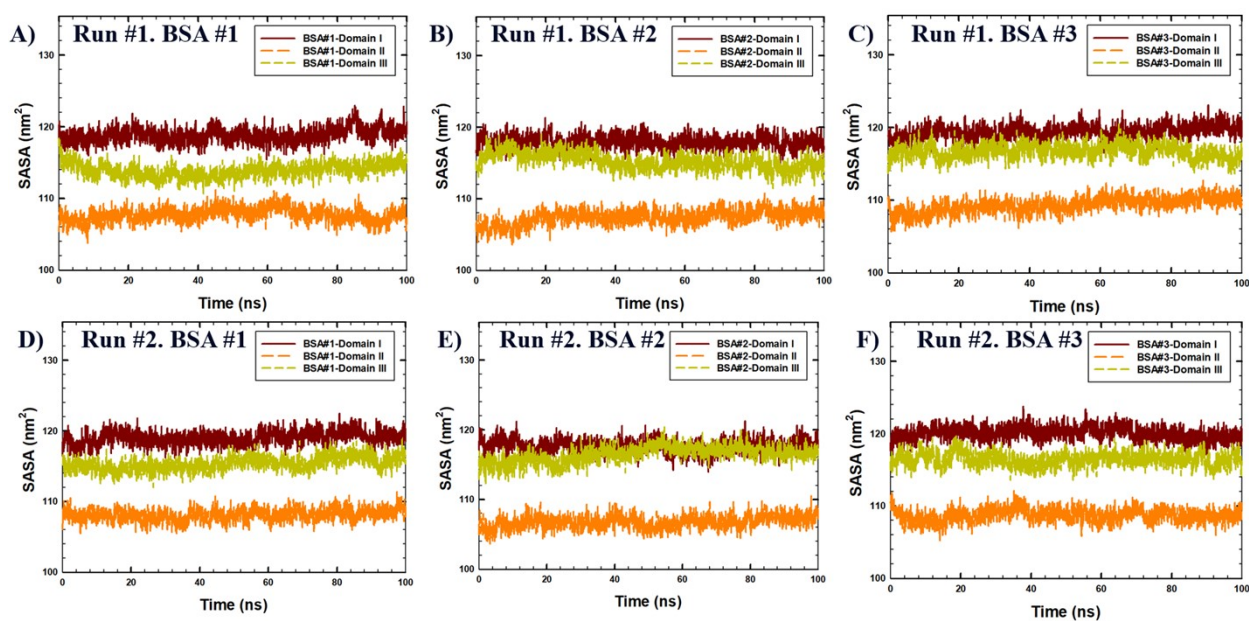


Figure S2. The solvent-accessible surface area of three BSA monomers: A-C) Run #1, D-F) Run#2

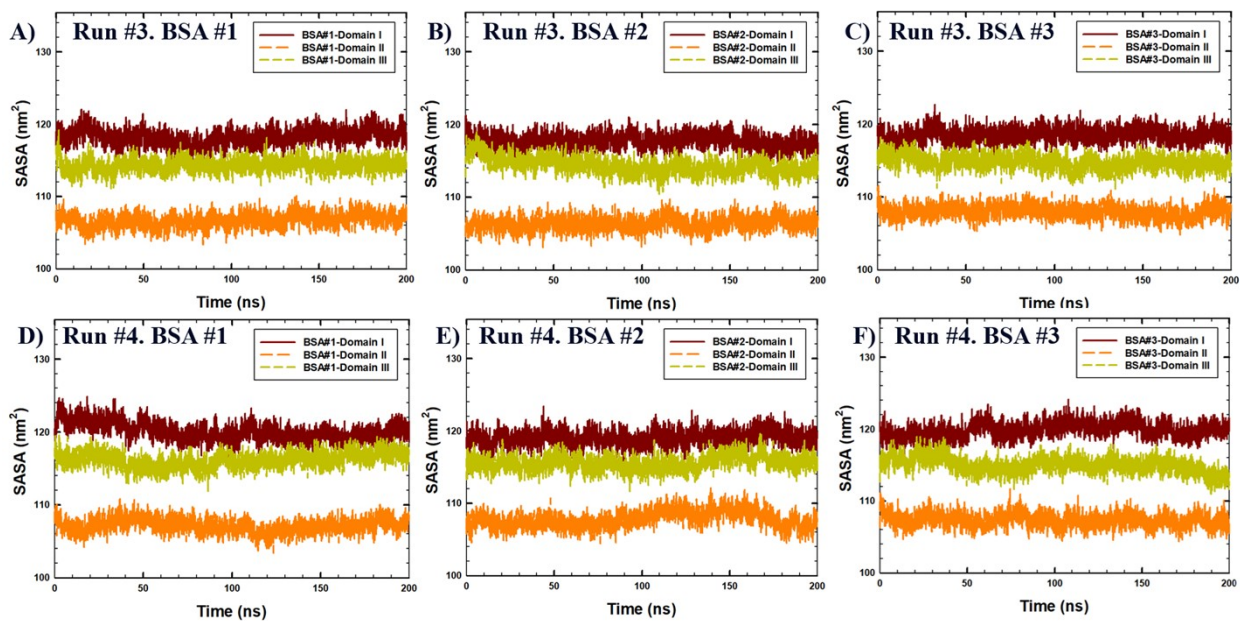


Figure S3. The solvent-accessible surface area of three BSA monomers: A-C) Run #3, D-F) Run#4