

# **Effect of gold nanoparticles on the conformation of bovine serum albumin: Insights from CD spectroscopic analysis and molecular dynamics simulations**

## **Supporting Information**

Samal Kaumbekova<sup>1,2§</sup>, Naoya Sakaguchi<sup>3§</sup>, Dhawal Shah<sup>2</sup>, and Masakazu Umezawa<sup>1,3\*</sup>

<sup>1</sup>Department of Medical and Robotic Engineering Design, Faculty of Advanced Engineering, Tokyo University of Science, 6-3-1 Niijuku, Katsushika, Tokyo 125-8585, Japan.

<sup>2</sup>Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr 53, Astana, 010000, Kazakhstan.

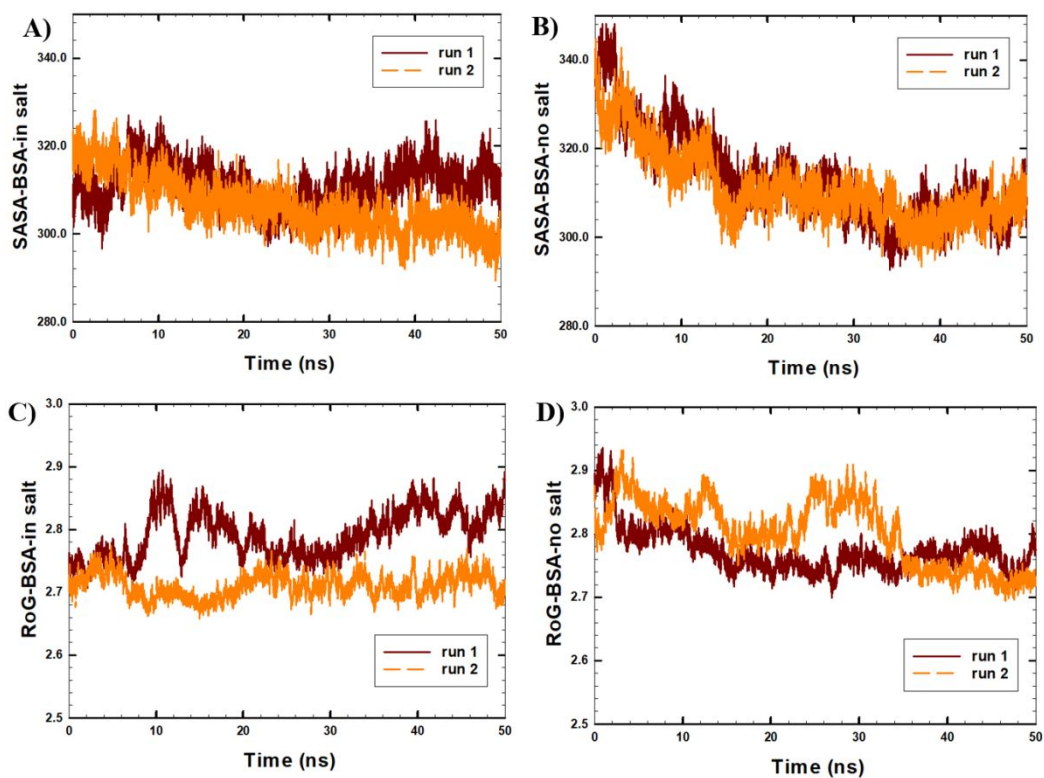
<sup>3</sup>Department of Materials Science and Technology, Graduate School of Advanced Engineering, Tokyo University of Science, 6-3-1 Niijuku, Katsushika, Tokyo 125-8585, Japan.

**Key Words:** gold nanoparticle; serum albumin; protein secondary structure; spectroscopic analysis; molecular dynamics simulations, protein corona

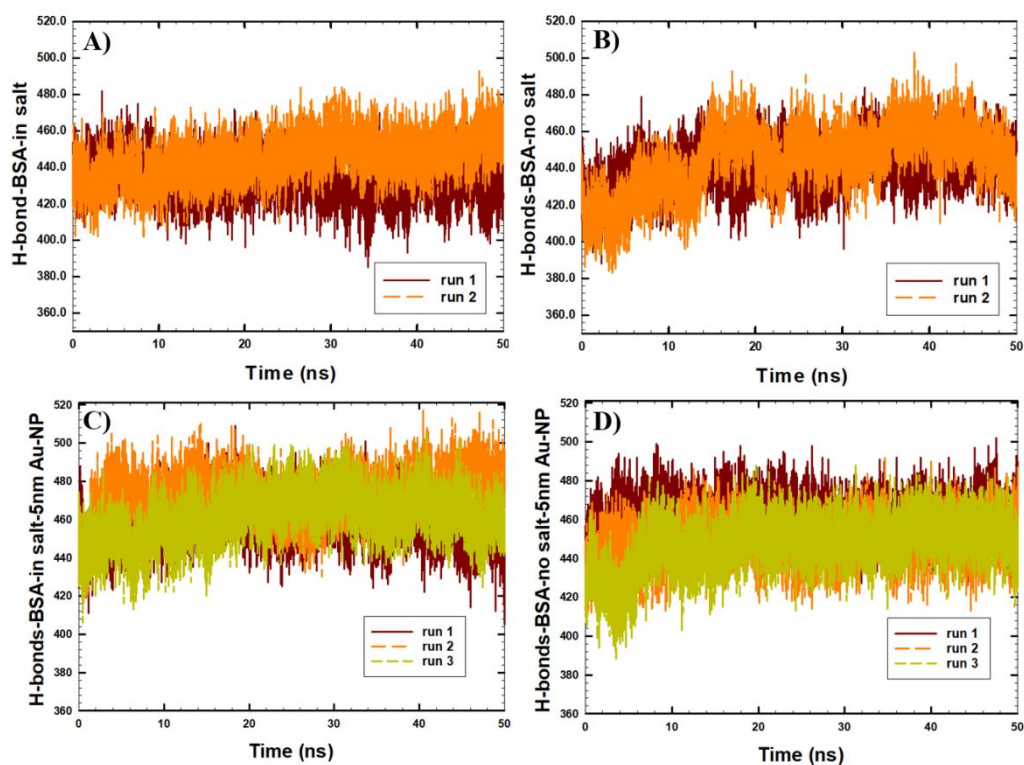
<sup>§</sup>These authors contributed equally

\*Corresponding author: Masakazu Umezawa, Tokyo University of Science, 6-3-1 Niijuku, Katsushika, Tokyo 125-8585, Japan.

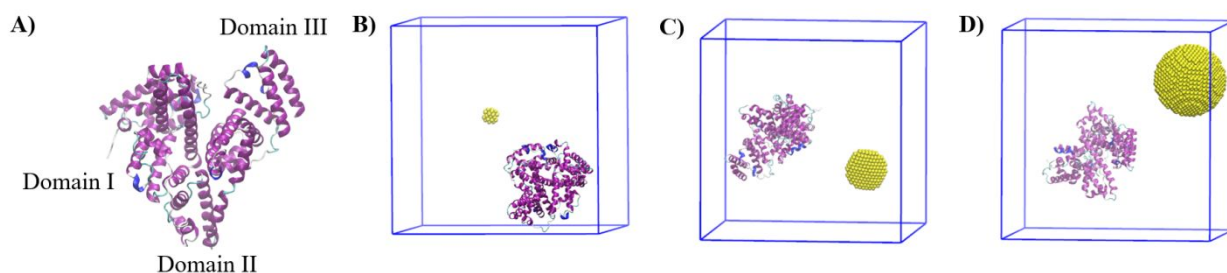
E-mail: [masa-ume@rs.tus.ac.jp](mailto:masa-ume@rs.tus.ac.jp)



**Figure S1.** Time evolution of A) total SASA of the BSA monomer in the presence of 0.15 M NaCl, B) total SASA of the BSA monomer in the absence of salt, C) RoG of the BSA monomer in the presence of 0.15 M NaCl, D) RoG of the BSA monomer in the absence of salt.



**Figure S2.** Time evolution of the intraprotein H-bonds A) in the system with no Au-NP, in the presence of 0.15 M NaCl, B) in the system with no Au-NP, in the absence of salt, C) in the system with 5-nm Au-NP, in the presence of 0.15 M NaCl, D) in the system with 5-nm Au-NP, in the absence of salt.



**Figure S3.** Representative snapshots of the initial structures at the beginning of the simulations (water and ions are not shown): A) BSA monomer, B) BSA monomer and 1-nm Au-NC, C) BSA monomer and 3-nm Au-NP, D) BSA monomer and 5-nm Au-NP.

**Table S1.** The average number of molecules in the simulated systems with BSA monomer in the absence and the presence of Au-NS: \*in the presence of 0.15 M NaCl, \*\*in the absence of salt.

*System	BSA	Au-NS	BSA: Au-NS mass ratio	H <sub>2</sub> O	Na <sup>+</sup>	Cl <sup>-</sup>
BSA	1	0	-	105171	321	305
BSA + 1-nm Au-NC	1	1	1 : 0.12	105179	321	305
BSA + 3-nm Au-NP	1	1	1 : 2.55	104583	321	305
BSA + 5-nm Au-NP	1	1	1 : 11.73	102783	321	305

**System	BSA	Au-NS	BSA: Au-NS mass ratio	H <sub>2</sub> O	Na <sup>+</sup>	Cl <sup>-</sup>
BSA	1	0	-	105754	16	-
BSA + 1-nm Au-NC	1	1	1 : 0.12	105771	16	-
BSA + 3-nm Au-NP	1	1	1 : 2.55	105235	16	-
BSA + 5-nm Au-NP	1	1	1 : 11.73	103433	16	-