

Supporting Information for

Photostable Single-molecule Nanoparticle Optical Biosensors for Real-time Sensing of Single Cytokine Molecules and their Binding Reactions

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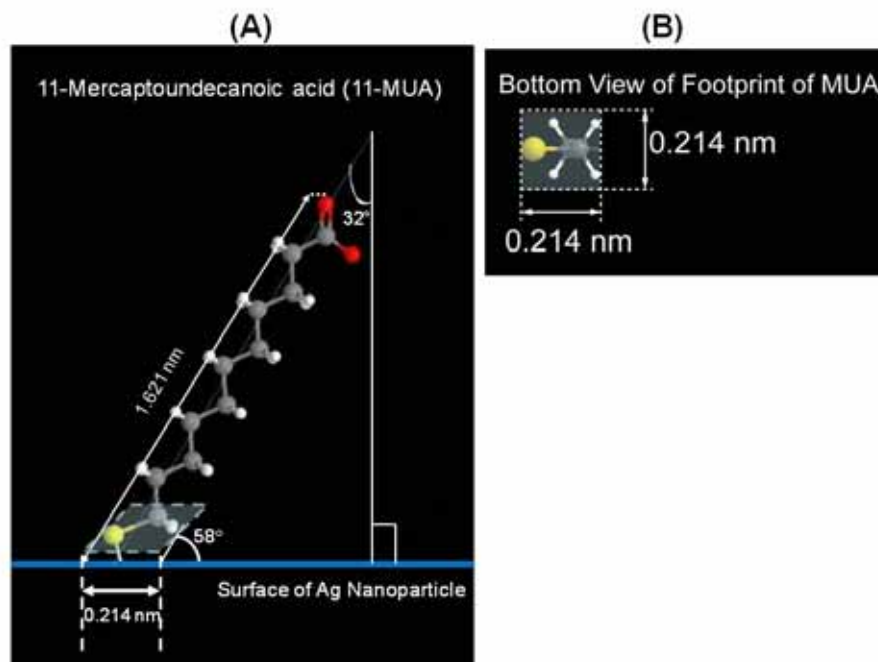


Figure 1S: Three-dimension (3D) molecular structure of 11-MUA anion shows the length and width of molecule at 1.621 nm and 0.214 nm, respectively: (A) MUA is tilted on the surface of Ag nanoparticle with anchoring angle of 58° and its thiol group is attached with Ag nanoparticle; (B) bottom view of footprint of MUA on the surface of nanoparticle. The molecular structures were created using Chem3D pro with energy optimization using MM2 and in water solvent under 25 °C and 1 atmosphere.

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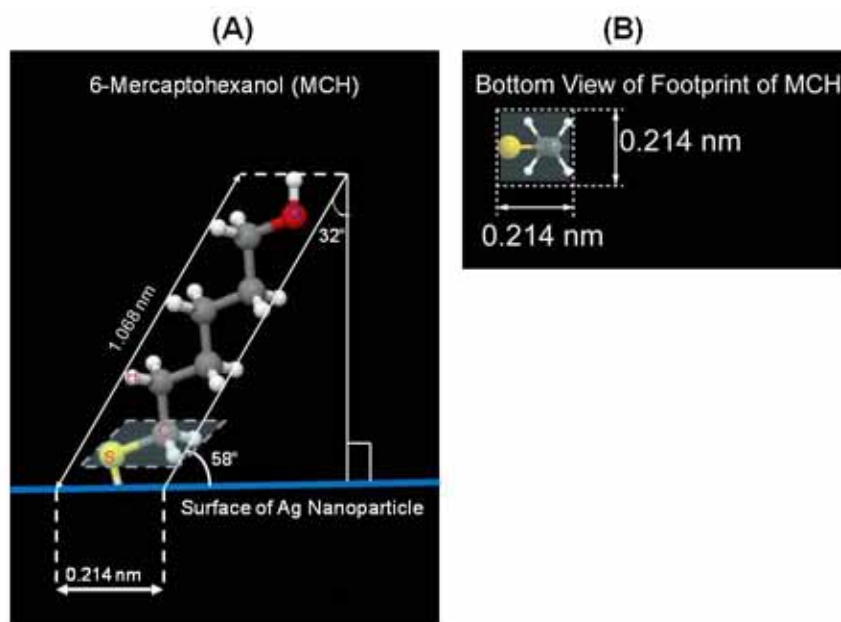


Figure 2S: Three-dimension (3D) molecular structure of 6-Mercaptohexanol (MCH) shows the length and width of molecule at 1.068 nm and 0.214 nm, respectively: (A) MCH is tilted on the surface of Ag nanoparticles with anchoring angle of 58° and its thiol group is attached with surface of Ag nanoparticle; (B) bottom view of footprint of MCH on the surface of nanoparticles. The molecular structures were created using Chem3D pro with energy optimization using MM2 and in water solvent under 25°C and 1 atmosphere. The oxygen in the hydroxyl group is assumed protonated.

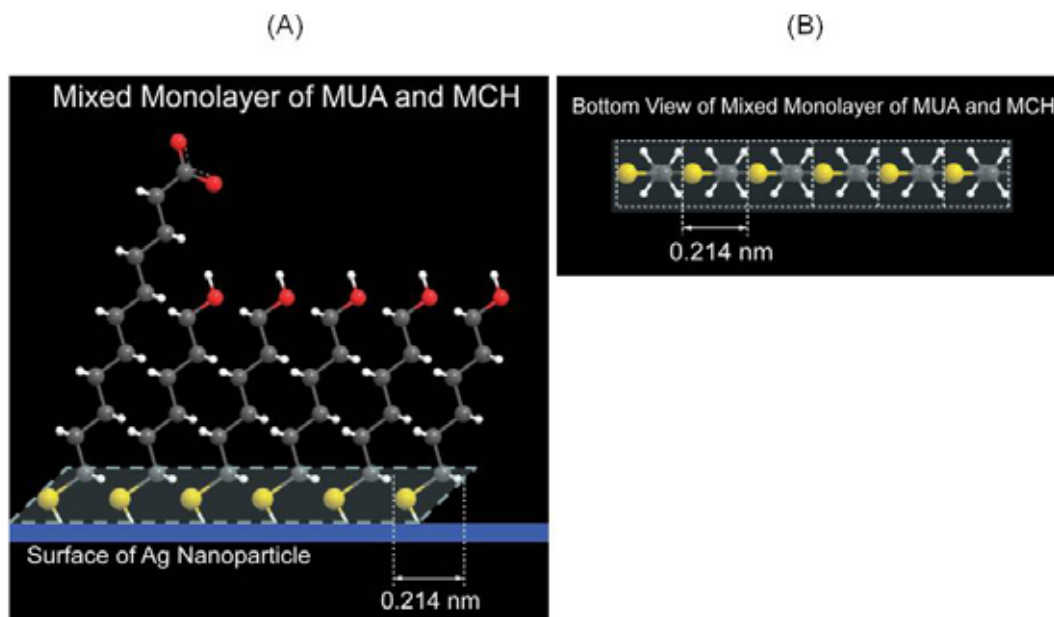


Figure 3S: Illustration of mixed monolayer of self-assembly of MUA and MCH molecules on the surface of nanoparticle, indicating the footprint area of individual molecule of $0.214\text{ nm} \times 0.214\text{ nm} = 0.0458\text{ nm}^2$.

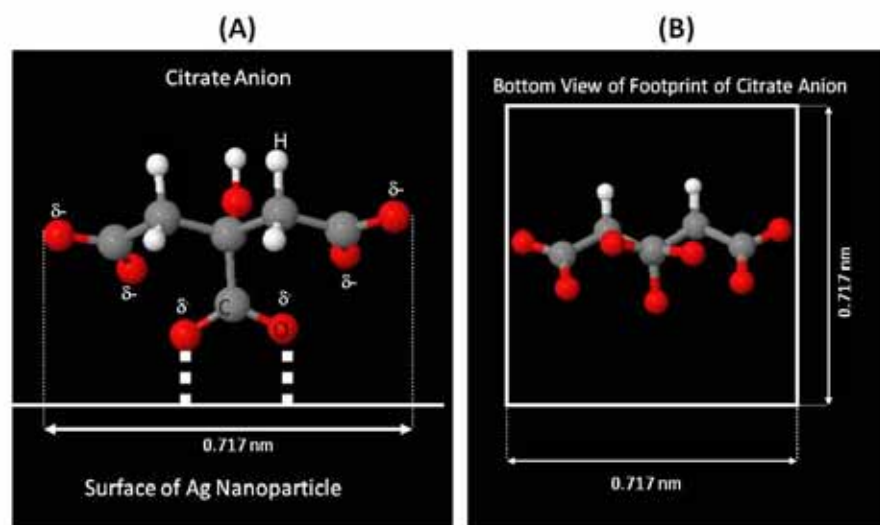


Figure 4S: Three-dimension (3D) molecular structure of citrate anion shows the length of molecule at 0.717 nm: (A) one carboxyl group of citrate anion is attached with the surface of Ag nanoparticles, allowing the molecule sit on the surface of nanoparticle; (B) bottom view of footprint of citrate anion on the surface of nanoparticles. Using the closing-pack model, we calculated the square of length of citrate molecules as its footprint (0.514 nm^2) on the surface of Ag nanoparticle. The molecular structures were created using Chem3D pro with energy optimization using MM2 and in water solvent under 25°C and 1 atmosphere. In comparison with molecular structures in Figures 5S and 6S where two and three carboxyl groups were attached on the surface of nanoparticles, the molecular structure in Figure 4S offers the lowest conformation energy, which was selected as a favorable conformation to calculate the footprint area of citrate on the surface of nanoparticles.

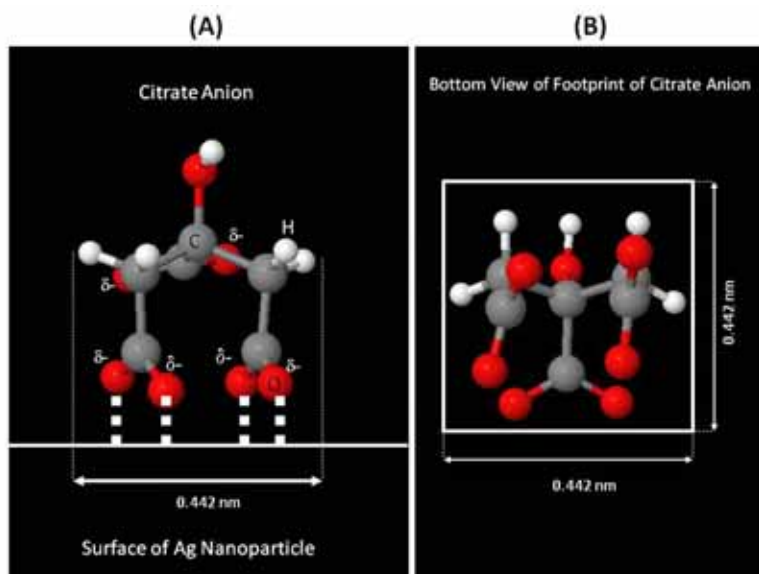


Figure 5S: Three-dimension (3D) molecular structure of citrate anion shows the length of molecule at 0.442 nm: (A) two carboxyl groups of citrate anion are attached with the surface of Ag nanoparticles, allowing the molecule sit on the surface of nanoparticle; (B) bottom view of footprint of citrate anion on the surface of nanoparticles in (A). Using the closing-pack model, we calculated the square of length of citrate molecules as its footprint (0.195 nm^2) on the surface of Ag nanoparticle. The molecular structures were created using Chem3D pro with energy optimization using MM2 and in water solvent under 25°C and 1 atmosphere.

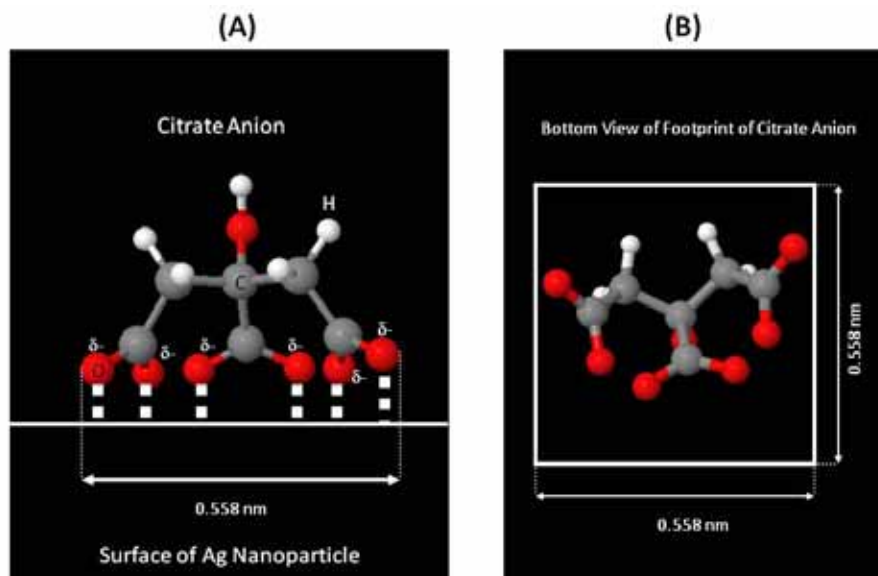


Figure 6S: Three-dimension (3D) molecular structure of citrate anion shows the length of molecule at 0.558 nm: (A) three carboxyl groups of citrate anion are attached with the surface of Ag nanoparticles, allowing the molecule sit on the surface of nanoparticle; (B) bottom view of footprint of citrate anion on the surface of nanoparticles in (A). Using the closing-pack model, we calculated the square of length of citrate molecules as its footprint (0.311 nm^2) on the surface of Ag nanoparticle. The molecular structures were created using Chem3D pro with energy optimization using MM2 and in water solvent under 25°C and 1 atmosphere.