

Supplementary Materials: Synthesis of Au NP@MoS₂ Quantum Dots Core@Shell Nanocomposites for SERS Bio-Analysis and Label-Free Bio-Imaging

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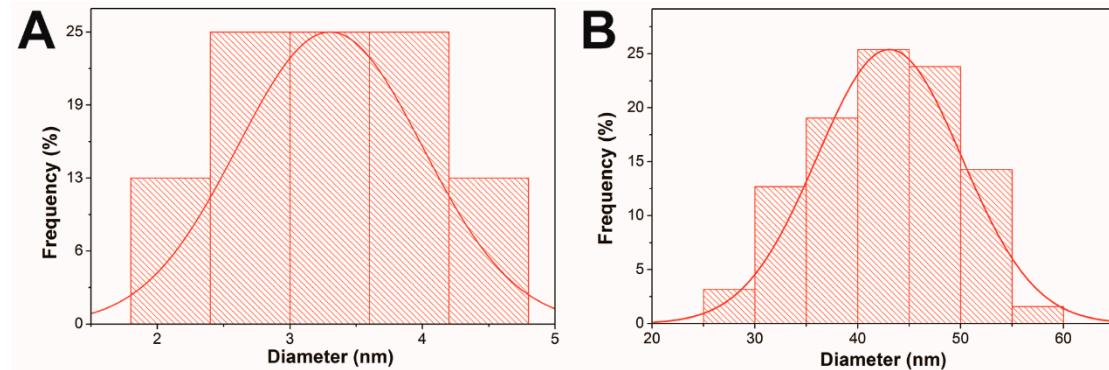


Figure S1. The mean diameter of MoS₂ QDs (A) and Au NP@ MoS₂ QDs (B), respectively.

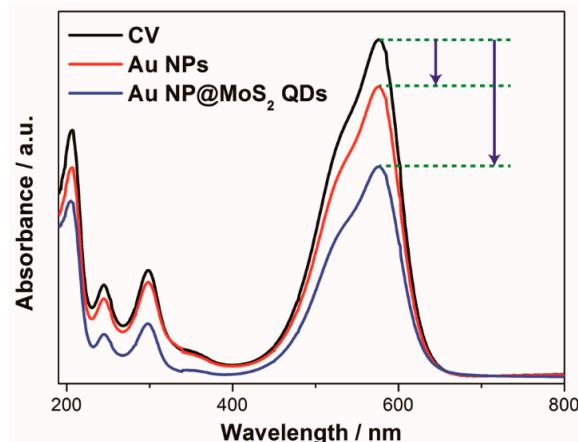


Figure S2. UV-Vis spectra of a 1 mM CV solution, and the remaining solution of 1 mM CV after the adsorption by 1 mM Au NPs or Au NP@MoS₂ QDs.

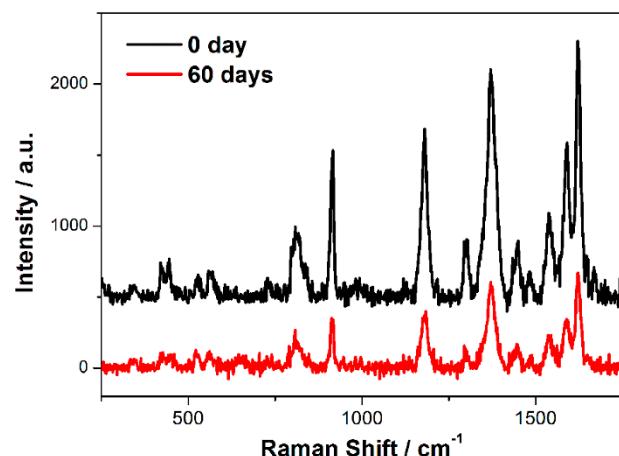


Figure S3. The stability of Au NPs.

Table S1. The assignments of the Raman bands of 4T1 cells incubated with AuNPs.

| Raman Shift (cm ⁻¹) 4T1 | Tentative assignment |
|--|---|
| 749 | T (d); Trp ring breath (p) |
| 835 | Tyr ring breath (p); O-P-O asym str (d) |
| 1008 | Phe ring sym breath (p) |
| 1136 | Proline(p) |
| 1320 | G(d), CH def (p) |
| 1353 | CH2/CH3 wag (p) |
| 1556 | Amide II(p) |
| 1646 | Amide I(p) |

Abbreviations: p, protein; l, lipid; d, DNA/RNA; Tyr, tyrosine; Trp, Tryptophan; T, thymine; G, guanine; str, stretching; breath, breathing; wag, wagging; sym, symmetrical; asym, asymmetrical; bk, backbone.

Table S2. The assignments of the Raman bands of 4T1 cells incubated with AuNP@MoS₂ QDs.

| Raman Shift (cm ⁻¹) 4T1 | Tentative assignment |
|--|--|
| 636 | Tyr, COO- bend or C-S str (p) |
| 655 | C-C twist Tyr (p) |
| 685 | G(d) |
| 703 | Cholesterol (l) |
| 749 | T (d); Trp ring breath (p) |
| 820 | Tyr ring breath (p) |
| 835 | Tyr ring breath (p); O-P-O asym str (d) |
| 930 | C-C bk str α helix (p); C-O-C glycos (c) |
| 976 | Trp, Tyr ring def (p) |
| 1010 | Phe ring sym breath (p) |
| 1069 | C-N str (p); Chain C-C str (l) |
| 1130 | C-N str (p); Chain C-C str (l); Disaccharide: C-O/C-C (c) |
| 1168 | C-C/C-N str (p) |
| 1224 | Amide III random coils (p) |
| 1276 | Amide III α helix (p), CH ₂ /CH ₃ def (p, l) |
| 1316 | G(d), CH def (p) |
| 1340 | CH ₂ /CH ₃ twist, CH ₂ /CH ₃ wag (p) |
| 1353 | CH ₂ /CH ₃ wag (p) |
| 1420 | CH ₃ asym str (p, l) |
| 1479 | G, A (d) |
| 1489 | A(d) |
| 1554 | Amide II (p) |
| 1572 | Amide II, Trp (p) |
| 1600 | Phe, Tyr (p) |

Abbreviations: p, protein; l, lipid; d, DNA/RNA; c, carbohydrate; Tyr, tyrosine; Trp, Tryptophan; Phe, phenylalanine; A, adenine; T, thymine; G, guanine; str, stretching; def, deformation; twist, twisting; breath, breathing; wag, wagging; sym, symmetrical; asym, asymmetrical; bk, backbone.