

## Electronic Supplementary Information

### Bacteria-induced Aggregation of Bioorthogonal Gold Nanoparticles for SERS Imaging and Enhanced Photothermal Ablation of Gram-positive Bacteria

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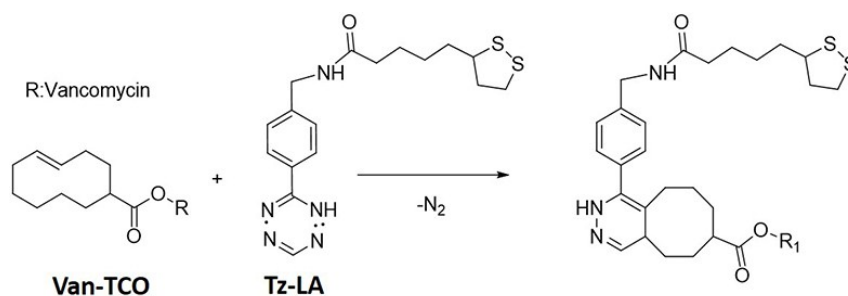


Figure S1. Cycloaddition reaction of trans-cyclooctene derivative of vancomycin (Van-TCO) and tetrazine derivative of liponic acid (Tz-LA)

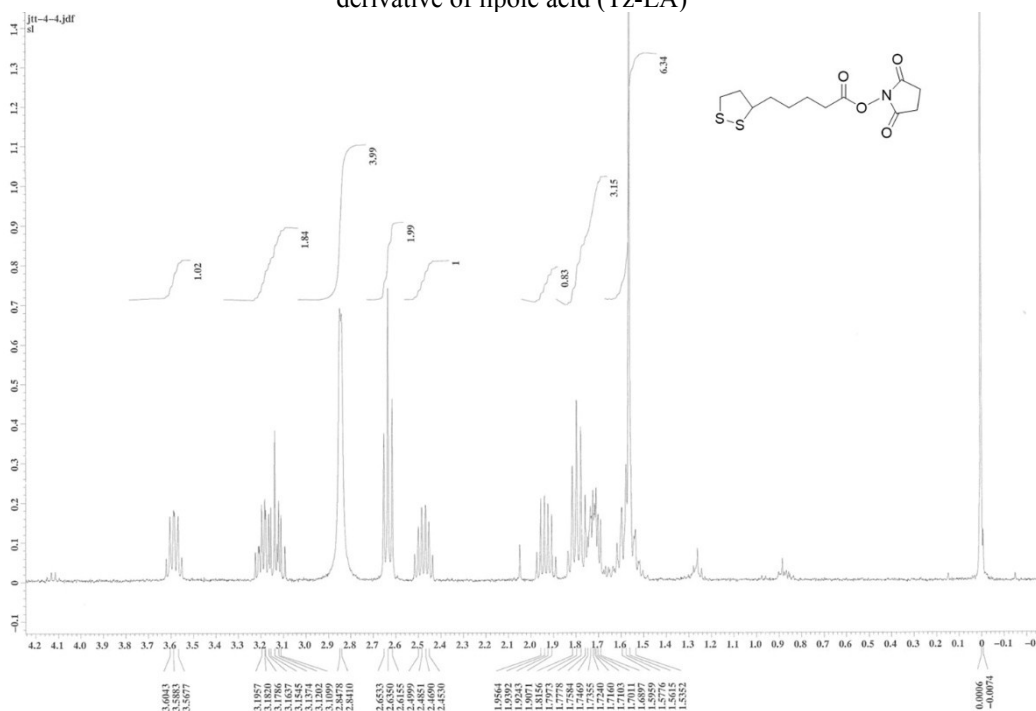


Figure S2. Nuclear magnetic resonance (NMR) data of liponic acid NHS-ester (LA-NHS)

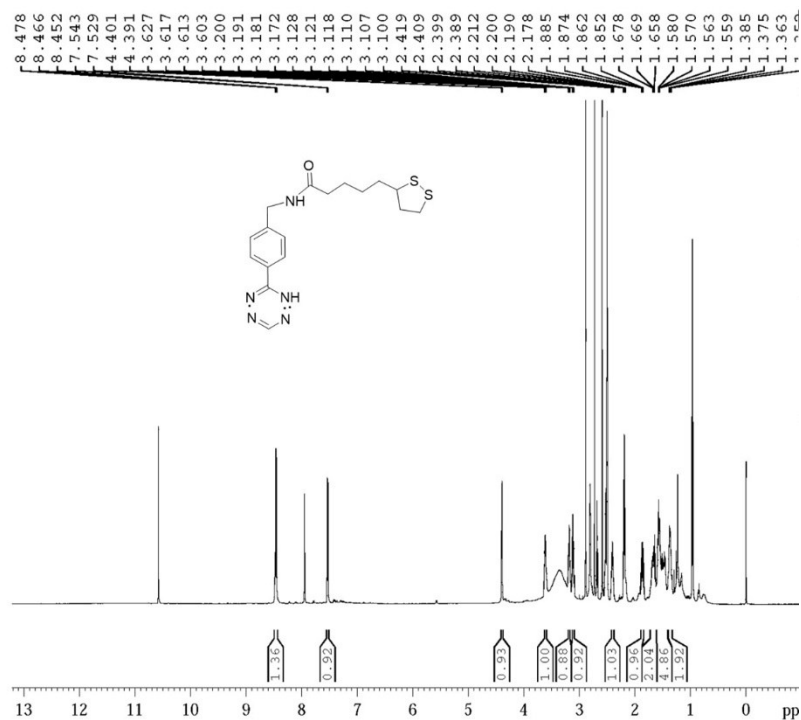


Figure S3. Nuclear magnetic resonance (NMR) data of tetrazin derivative of lipoic acid (Tz-LA)

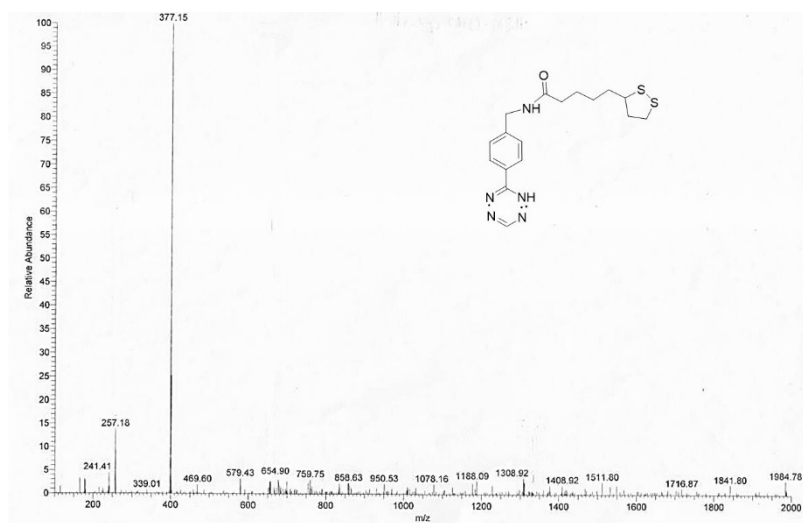


Figure S4. Liquid chromatography-mass spectrometry (LC-MS) data of tetrazin derivative of lipoic acid (Tz-LA)

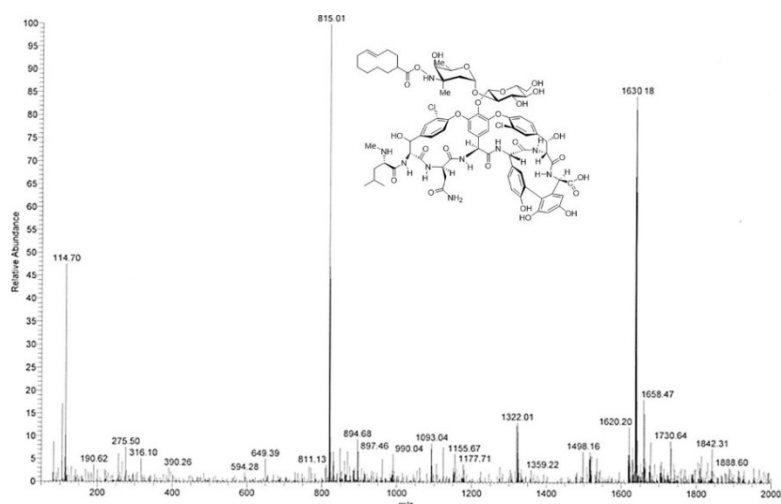


Figure S5 Liquid chromatography-mass spectrometry (LC-MS) data of trans-cyclooctene derivative of vancomycin (Van-TCO)

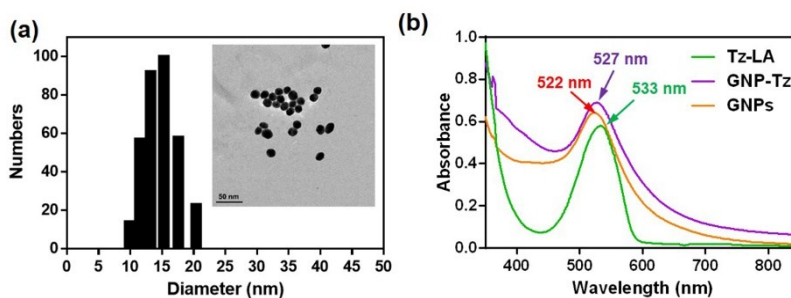


Figure S6. Characterizations of gold nanoparticles using transmission electron microscopy (TEM), dynamic light scattering (DLS) (a) and UV-Vis spectroscopy (b)

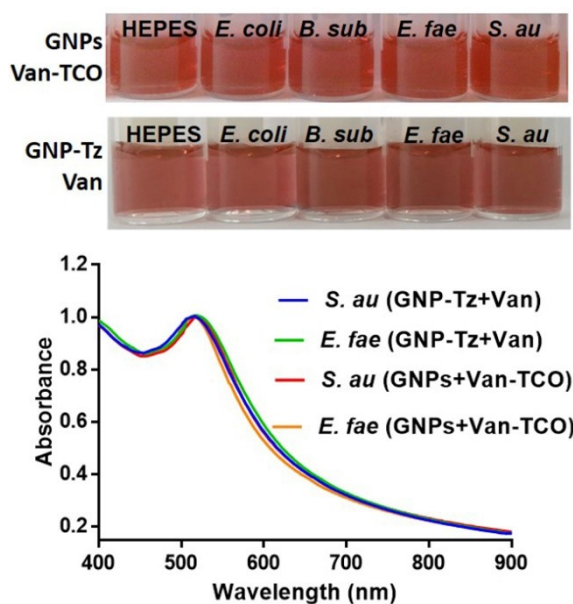


Figure S7. (a) Photographs of various bacterial strains treated with GNPs/Van-TCO and GNP-Tz/Van; (b) UV-vis spectra of two pathogens (*S. au* and *E. fae*) above mentioned.

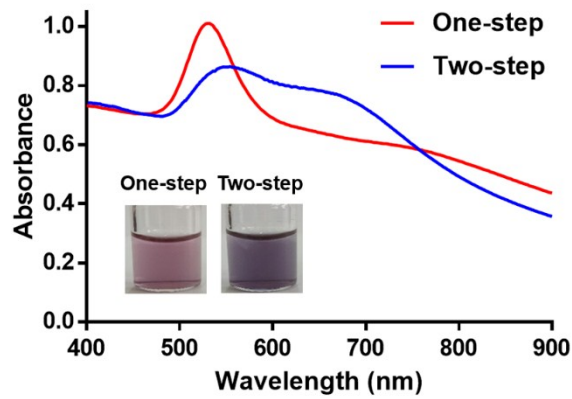


Figure S8. UV-vis spectra of *B. sub* bacterial strain following the two-step cycloaddition labelling method compared to that following the one-step labelling method. The embedding graphs are the digital images of samples above mentioned.

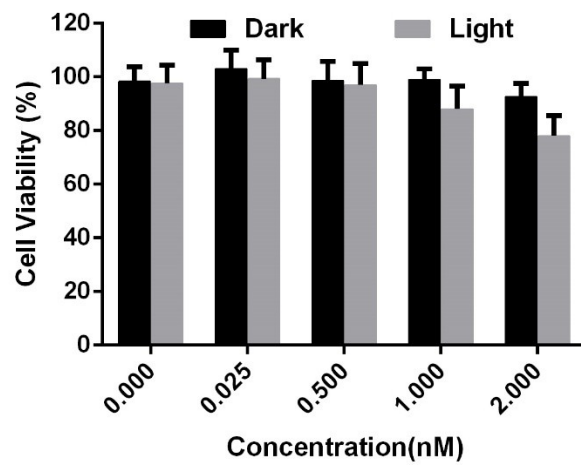


Figure 9. Cytotoxic and photocytotoxic effect of GNP-Tz toward 3T3 fibroblasts cells treated with Van-TCO. The results were mean values  $\pm$  SD of triplicate experiments.

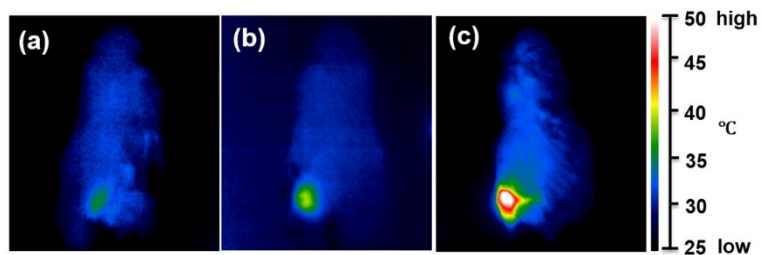


Figure S10. Thermographic images of infection sites treated by Van-TCO (a), GNP-Tz (b) and Van-TCO together with GNP-Tz (c) after NIR light treatment.