Supplementary Information

Preferential Accumulation of Phospholipid-PEG and Cholesterol-PEG Decorated Gold Nanorods into Human Skin Layers and their Photothermal-Based Antibacterial Activity

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Figure S1. ¹H-NMR spectra of DSPE-PEG-SH, DSPE-PEG-GNR and CTAB-GNR. Combined ¹H-NMR spectra of **A.** DSPE-PEG-SH and **B.** DSPE-PEG-GNR show the signals similarity of characteristic chemical shift values with slightly broadened and shifted peaks upon attachment to GNR; (a) a characteristic sharp peak of repeated units of PEG at ~ 3.68 ppm; (b) a characteristic sharp peak of methylene groups of DSPE at ~ 1.25 ppm; (c) a characteristic peak of the methyl group of DSPE at ~ 0.89 ppm; (d) a characteristic peak of the methylene groups attached to amide at 1.60 ppm. **C.** ¹H-NMR spectrum of CTAB-GNR showed a

characteristic sharp peak of the γ -methyl protons at ~ 3.39 ppm that was reduced dramatically upon displacement of CTAB by DSPE-PEG-SH. All the spectra were acquired in CDCL₃.



Figure S2. ¹H-NMR spectra of Chol-PEG-SH, Chol-PEG-GNR and CTAB-GNR. Combined ¹H-NMR spectra of **A.** Chol-PEG-SH and **B.** Chol-PEG-GNR show the signals similarity of characteristic chemical shift values with slightly broadened and shifted peaks upon attachment to GNR; (a) a characteristic sharp peak of repeated units of PEG at ~ 3.68 ppm; (b)

Characteristic peaks of cholesterol protons. C. ¹H-NMR spectrum of CTAB-GNR showed a characteristic sharp peak of γ -methyl protons at ~ 3.39 ppm that was reduced dramatically upon displacement of CTAB by Chol-PEG-SH. All the spectra were acquired in CDCL₃.



Figure S3. Confocal fluorescence microscopy images of skin samples pre-treated with m-PEG-GNR, NH₂-PEG-GNR and COOH-PEG-GNR. **A & B.** SC and dermis of skin pre-treated with m-PEG-GNR, respectively. **C & D.** SC and dermis of skin pre-treated with NH₂-PEG-GNR respectively. **E & F.** SC and dermis of skin pre-treated with COOH-PEG-GNR, respectively.

All the images showed low fluorescence intensity of the neutral or charged PEGylated GNR applied to skin samples. Scales = A, C and E = 200 μ m, B, D and F = 100 μ m.



Figure S4. Fluorescence intensities of GNR of different surface functionalities that accumulated into: A. Stratum corneum layers, and B. Dermis layer. Data are given as mean \pm SD (n = 3). Unpaired t-test was used to evaluate the differences; * p < 0.05, ** p < 0.01.