Electronic Supplementary Material (ESI) for Analyst.
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Electronic Supporting Information (ESI)

Magnetic–optical nanohybrid for targeted detection, separation, and photothermal ablation of drug-resistant pathogens

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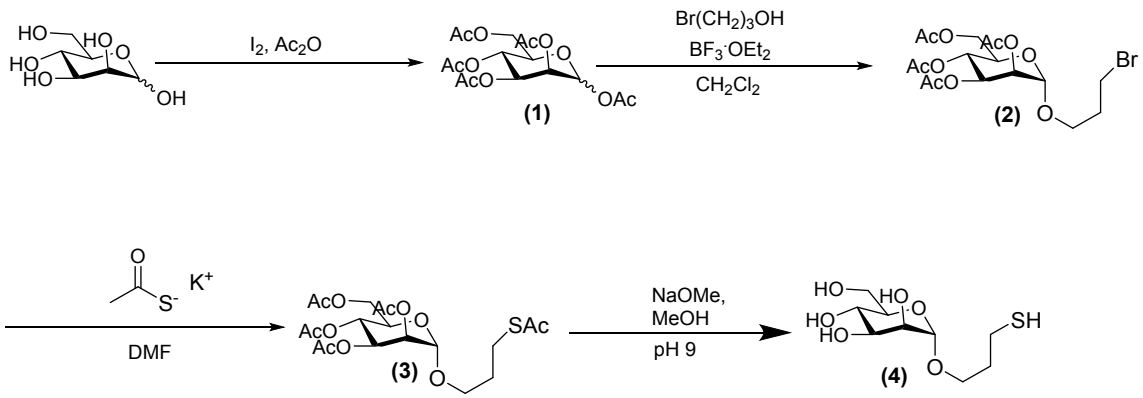
Materials and Methods: All chemicals and reagents were of analytical grade. Unless otherwise stated, all chemicals were obtained from Sigma-Aldrich and used without further purification.

Scheme S1: Scheme of Synthesis of Thiolated-Mannose and Experimental Details:



SI-1: 1,2,3,4,6-Penta-O-acetyl-D-mannopyranose (1). This compound was synthesized according to literature procedure.[1] D-Mannose (5.0 g, 27.8 mmol, 1.0 eq.) was slowly added to a solution of Iodine (I_2) 0.28 g, 1.1 mmol, 0.04 eq.) in Ac_2O (25 mL) at 0 °C and under a nitrogen atmosphere. After stirring for 30 min at 0 °C and an additional 16 h at r.t., the reaction mixture was diluted with 30 mL of CH_2Cl_2 and washed with a cold saturated aqueous solution of

Na_2SO_3 (2 x 30 mL), then with a saturated aqueous solution of $NaHCO_3$ (4 x 18 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford compound **(1)** as clear viscous liquid (yield 91%).

(3′-bromopropyl)-2,3,4,6-tetra-O-acetyl-D-mannopyranoside (2). This compound was synthesized according to modified literature procedure.[2] Compound 1 (3.33 g, 8.53 mmol) was dissolved in dry CH_2Cl_2 (20 mL) under N_2. To this solution, 3-bromo-1-propanol (1.55 cm^3, 17 mmol) was added and the mixture was cooled on an ice bath. Boron trifluoride etherate (4.4 cm^3, 35.0 mmol) was added dropwise for 20 min. The reaction mixture was left to attain room temperature and was stirred in the dark under a nitrogen atmosphere for 48 h. The solution was then diluted with ice-cold water and extracted twice with CH_2Cl_2.The organic phase was washed with aqueous saturated sodium bicarbonate solution (40 cm^3), water (40 cm^3), and aqueous saturated sodium chloride. The combined organic layers were dried over sodium sulfate, filtered and concentrated under reduced pressure. The resulting oil was then purified using column chromatography on silica gel (ethyl acetate/hexane (1:3, v/v)). The relevant fractions were collected, combined and concentrated under reduced pressure to yield 3′-bromopropyl-2,3,4,6-tetra-O-acetyl-D-mannopyranoside **(2)** as a dark yellow oil.

3′-acetylthiopropyl 2,3,4,6-tetra-O-acetyl-D-mannopyranoside (3). Compound **(3)** was synthesized according to modified literature procedure.[2, 3] Potassium thioacetate (0.45 g, 4.0 mmol) was added to a solution of **2** (1.5 g, 3.2 mmol) in DMF (15 ml) at 0 ^{0}C. The mixture was stirred overnight at room temperature and then extracted with ethyl acetate. The organic phase was then washed with, water and brine, dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by chromatography (n-Hex/EtOAc, 3:2) to afford **3.**

(3-mercaptopropyl)-D-mannopyranoside (4) A flask was charged with **3** (1.0 g, 2.15 mmol) dissolved in anhydrous methanol (15 cm^3). To this solution sodium methoxide (0.12 g, 2.2 mmol) was added and the reaction mixture was stirred at room temperature under a nitrogen atmosphere.[3] TLC analysis using methanol: CH_2Cl_2 (1:9), showed that after 12 h the reaction had gone to completion. Amberlite IR-120H ion-exchange resin was washed with dry methanol and then added to the reaction mixture and stirred for 30 min. The resin was then filtered off under gravity and the resulting solution concentrated under vacuum. The residue was purified by chromatography (DCM/MeOH, 9:1) to afford **4** as a colorless solid. (Yield 0.31 g, 57%).[4]

Figure S1: NMR and MS of (4)

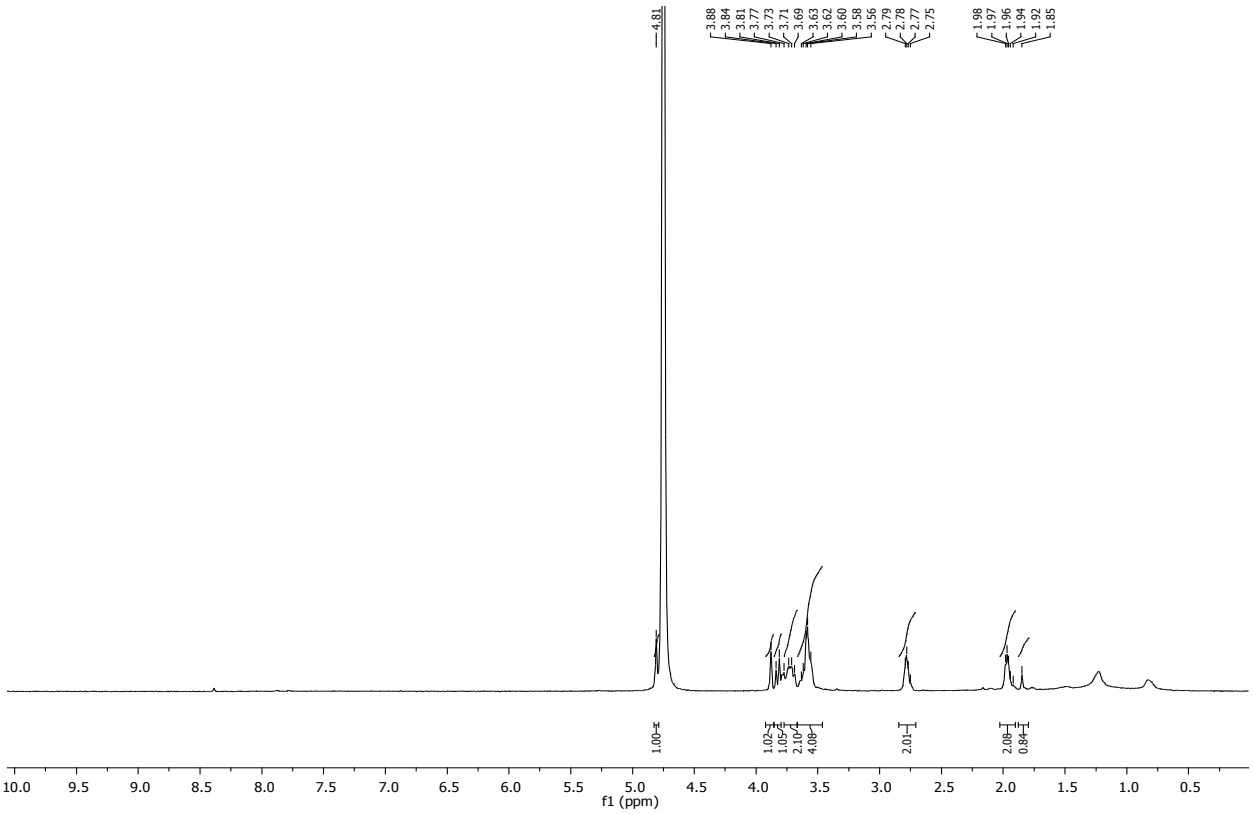


Figure S1a: ^1H NMR of thiolated mannose

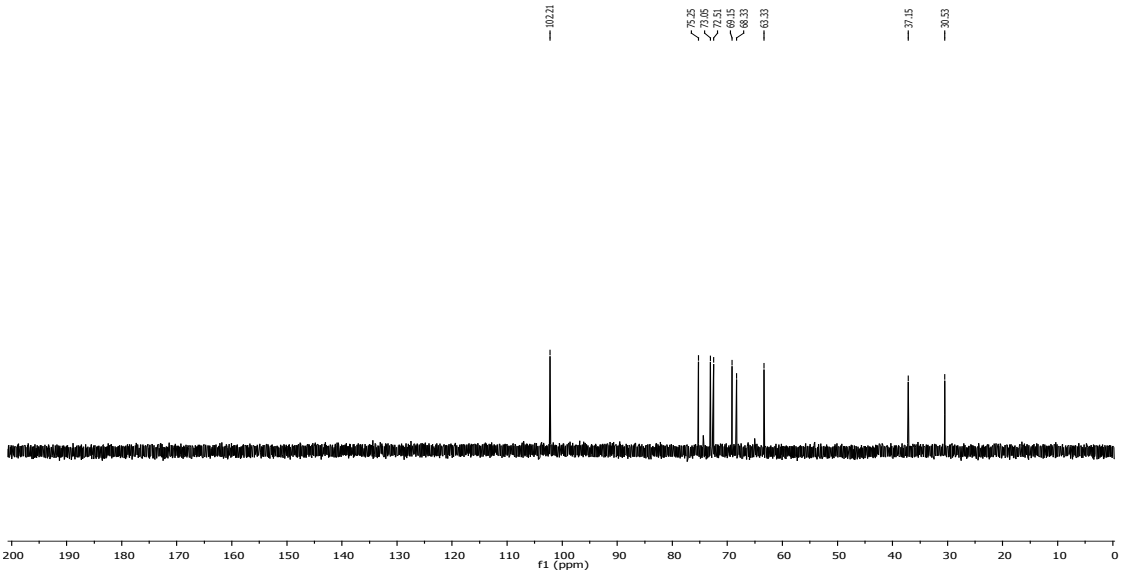


Figure S1b: ^{13}C NMR of thiolated mannose

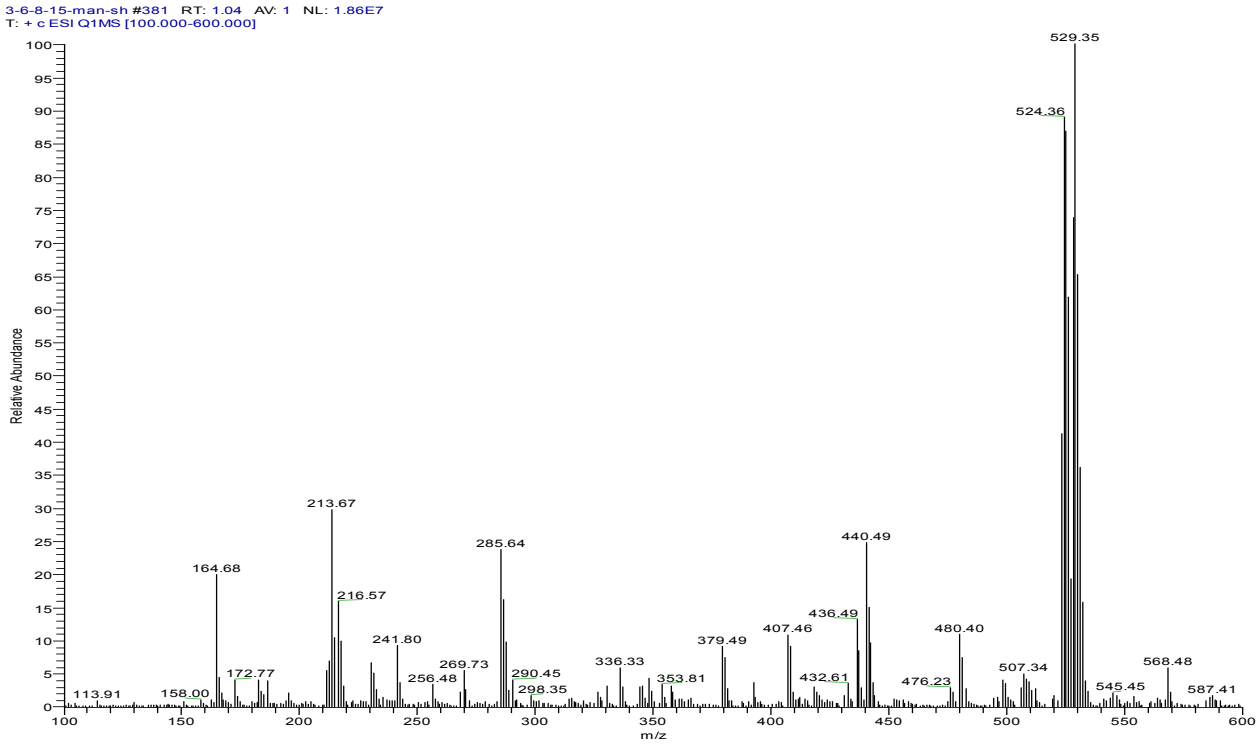


Figure S1c: MS of thiolated mannose

Compound 4: ^{1}H NMR (500 MHz, D_2O) δ 4.81 (br s, 1H), 3.88 (br m, 1H), 3.83 (d, *J* = 12.5 Hz, 1H) 3.77-3.69 (m, 2H), 3.63-3.56 (m, 4H), 2.79-2.75 (m, 2H), 1.98-1.92 (m, 2H), 1.85 (s, 1H –SH); **^{13}C NMR (125 MHz, D_2O)** δ 102.2, 75.2, 73.0, 72.5, 69.1, 68.3, 63.3, 37.1, 30.5. **MS (ESI$^+$)** *m/z* calculated for $[M+Na]^+$ $C_{18}H_{34}NaO_{12}S_2^+$ 529.14, found 529.35.

SI-2: DTNB-labeled con A loading onto mannose stabilized AuNP@SWCNTs.

The reporter DTNB molecules (0.04mM) and con A (52 µg mL^{-1}) were mixed at volume ratio 1:2 respectively. 150 µL of mixture was added to 1.5 mL of the mannose-stabilized AuNP@SWCNTs. Then the mixed solution was incubated for 10 min at 25 °C under gentle shaking and stood overnight at 4 °C without mixing. PEG was added to a final concentration of 0.5% (w/v) and incubated for 20 min at 25 °C. The mixture was centrifuged (4 000 rpm, 15 min, 4 °C, supernatant decanted) to remove the unbound con A, DTNB molecules and PEG, and rinsed with buffer. The centrifuging/rinsing procedure was repeated 2 times. The final deposition was suspended in 2 mL of buffer and stored at 4 °C for further use. The quality of the particles was monitored with UV−vis spectrophotometer and TEM.

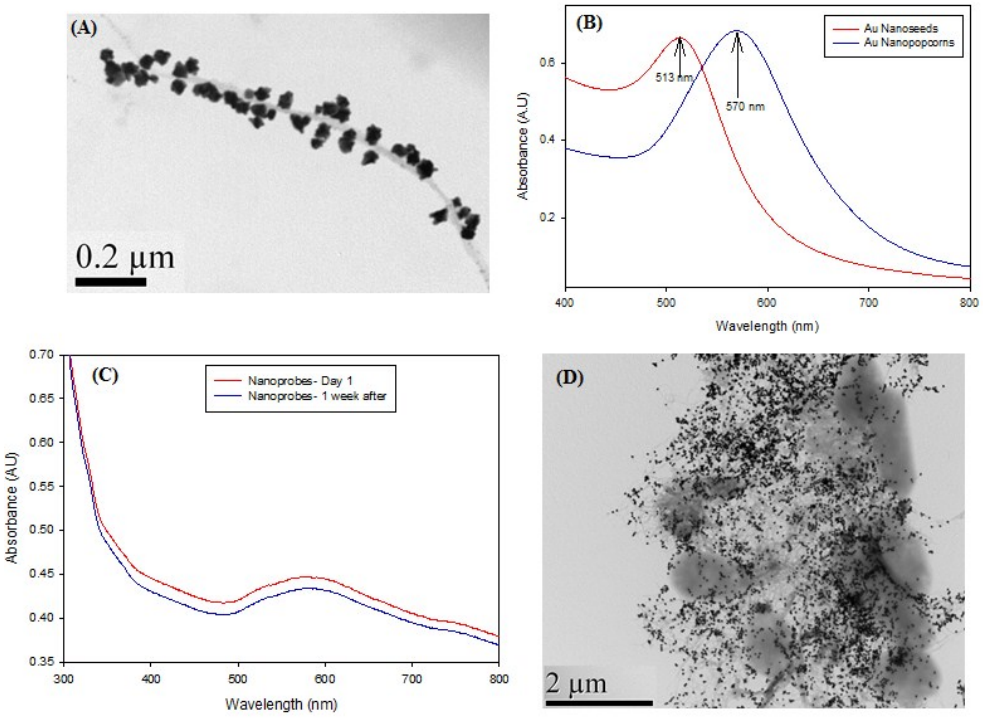


Figure S2. TEM images of (A) mannose-conjugated AuNP@SWCNTs, UV–vis spectra of (B) Au Nanoseeds (red line), Popcorn-shaped AuNPs (blue line) (C) Nanoprobes:- day 1(red line) and after 1 week (blue line), (D) TEM image of E. coli immobilized with reporter nanoprobes.

SI-3: Cell Viability Assays. For all of the cell studies, the *E. coli* cell culture was diluted with PBS before use. In order to evaluate the effect of the MNPs and DTNB-tagged Con A-AuNP@SWCNT nanostructures on the *E. coli* viability, 10 µL - 100 µL of mAb-MNP and 50 µL - 150 µL DTNB-tagged Con A-AuNP@SWCNT nanostructures dispersed in PBS was added to diluted cell culture (1.3×10^4 CFU/mL) and incubated at room temperature for 3 h before spreading 25 µL of the resulting mixture onto a LB agar plate. Similar tests were done with 150 µL of the nanostructures in the ratio 1:2, 1:3, 1:4 and 1:5 (mAb-MNP: DTNB-tagged Con A-AuNP@SWCNT). The agar plate containing the *E. coli* spread was cultured in an incubator at 37 °C overnight. The bacterial growth was evaluated through counting of the resulting colonies.

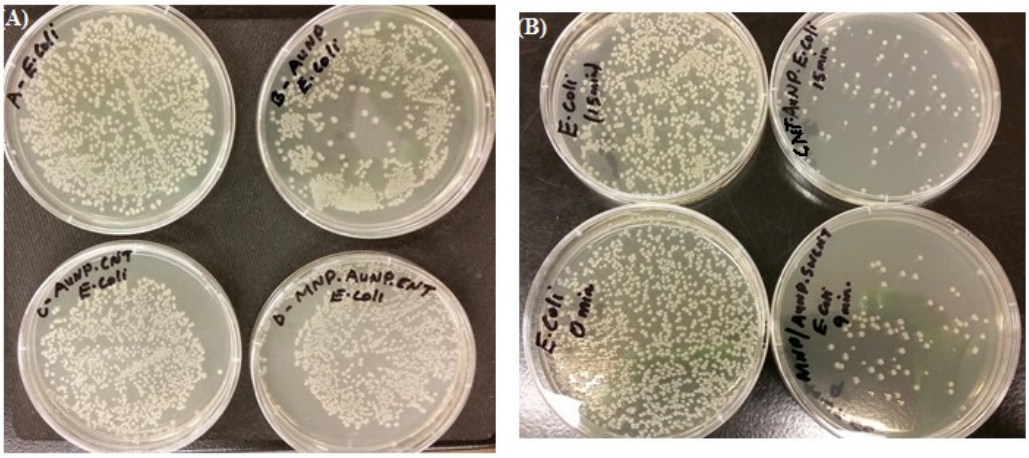


Figure S3. **(A):** Cytotoxicity studies showing high bacterial viability after different assay treatment (A-D), and **(B):** Comparison of photothermal effects of AuNP@SWCNT and AuNP@SWCNT/MNP, and untreated E. coli

SI-4: Photothermal Laser treatment, General procedure. 1.3×10^4 CFU/mL of *E. coli* samples (treated and untreated) was exposed in an optical cuvette to a 670 nm laser at 2.5 W/cm^2 power. Use of a 2-mm-pinhole in front of the cuvette provided a relatively uniform beam-intensity

profile and there was a relatively uniform exposure of the entire sample in the cuvette. 25 µL of the treated samples were plated in triplicate on agar plates and incubated at 37 °C for 18 hours.

V. REFERENCES

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