Supporting Information

Smartphone spectrometer for biosensing

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Method and Materials

Materials

2,2'-Azinobis(3-ethylbenzothiazoline-6-sulfonic Acid Ammonium Salt) (ABTS) was purchased from TCI America (USA). The peptide binder **TP** (CALNN-Peg_4-FYSHSFHENWPS) and peptide spacer (CALNN) used were customized and purchased from GL, Shanghai. Cardiac human Troponin I was obtained from Abcam, US. Triethylene glycol mono-11-mercaptoundecylether (Thiol-PEG, #673110) and other chemicals were purchased from Sigma-Aldrich. 60 nm gold nanoparticles were purchased from BBI solution (UK).

Smart phone spectrometer

A small chamber incorporate with a CD disk and a sample holder was made of plastic as shown in Fig. 1. The chamber was attached on the cell phone to fit the position of the LED light which pass through the sample in the chamber and diffracted to the CCD camera on the phone.

Glucose detection

A stock solution A with concentration of 50 mM ABTS and 25 U/ml HRP in water was prepared. Then, 0.5 mL of stock solution A was mixed with 0.5 ml of GOD at concentration of 5 U/ml, and

then added to 8 ml PBS buffer to form stock solution B. For the glucose detection, 0.2 ml of sample solution spiked with glucose at concentrations from 1 mM to 50 mM were added in the stock solution B. The absorbance was measured by smart phone spectrometer and the plate-reader (TECAN).

Synthesis of AuNPs

Gold nanoparticles with 16 nm and 36 nm were synthesized by citrate reduction method. Briefly 100 mL of 0.01% (0.1 mg/mL) gold(III) chloride trihydrate solution was boiled in a well-cleaned flask. After boiling 2.75 mL or 1.75 mL of sodium citrate was added into the flask in order to obtain 16 or 36 nm AuNPs, respectively. It was then kept boiling until the color changed from light yellow to red. The synthesized spherical gold nanoparticles were verified by DLS and stored in fridge until use.

Functionalization of AuNPs with peptides for Troponin I detection

The peptide spacer (2 mM) 12.5 μL and **TP** (1 mM) 25 μL were mixed in 500 μL phosphate buffered saline buffer (1×, 0.05% Tween) followed by adding of 1 mL AuNPs (36 nm). The AuNPs solution was incubated for overnight at room temperature. Afterwards, the functionalized AuNPs were purified and concentrated by repeated centrifugations. It was stored in fridge until use.

The microscopy imaging of the applied CD grating structure indicates the grating period about 1.56 μm and 640 lins/mm (Fig. S1).

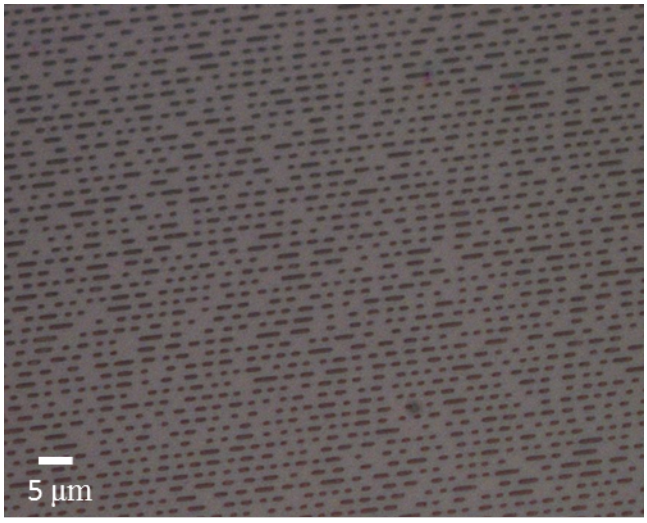


Fig. S1 The microscopy imaging of the CD grating structure.

Fig. S2 shows a photo of a 96-well plate containing ABTS/HRP/GO solution that is incubated with different concentration of glucose from 0 to 50 mM. The clear solution changes to blue color in the presence of glucose higher than 1 mM and its color intensity increase with the concentration of glucose.

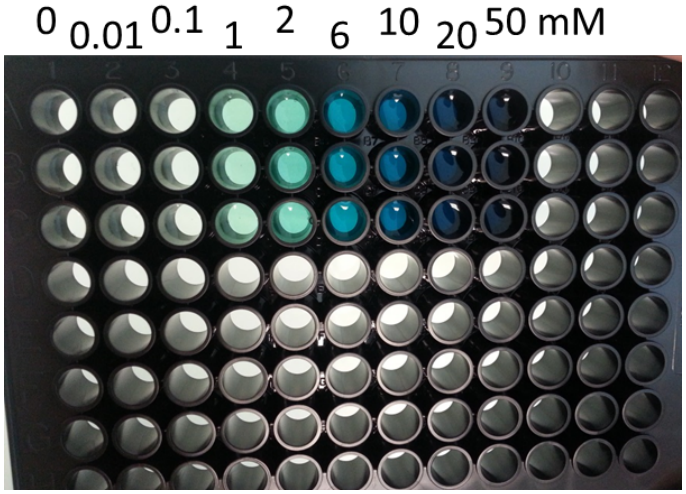


Fig. S2 A photo taken from a 96-well plate in which the colorimetric assay based on ABTS/HRP/GO solution was applied for the detection of glucose at concentration from 0 to 50 mM.

Fig. S3 shows the absorbance spectra of the ABTS/HRP/GO solution after the addition of glucose measured with plate-reader (Fig. S2A) and smartphone spectrometer (Fig. S2B), respectively. There is small difference at the wavelength around 550 nm, due to the worse linear sensitivity of the smartphone to light intensity at this wavelength range as compared with the detector in plate-reader.

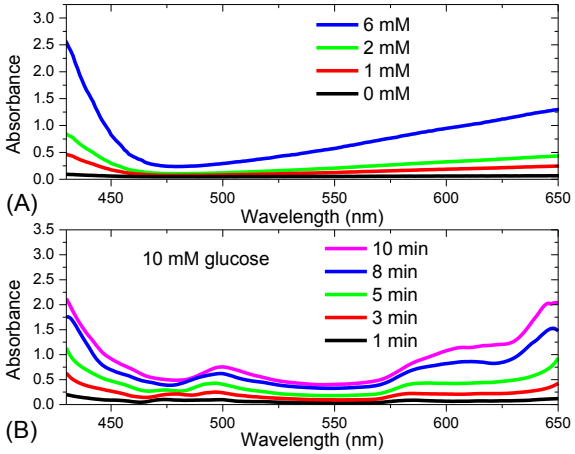


Fig. S3 (A) The absorbance spectra of the ABTS/HRP/GO solution measured 1 hour after adding 0 to 6 mM glucose, measured by TECAN plate-reader. (B) The absorbance spectra of the same solution measured after incubation of 10 mM glucose for 1 to 10 min, measured by smartphone.

Fig. S4 shows the spectra of AuNPs with diameter of 16, 36 and 60 nm, as measured by smartphone spectrometer and UV/Vis spectrometer.

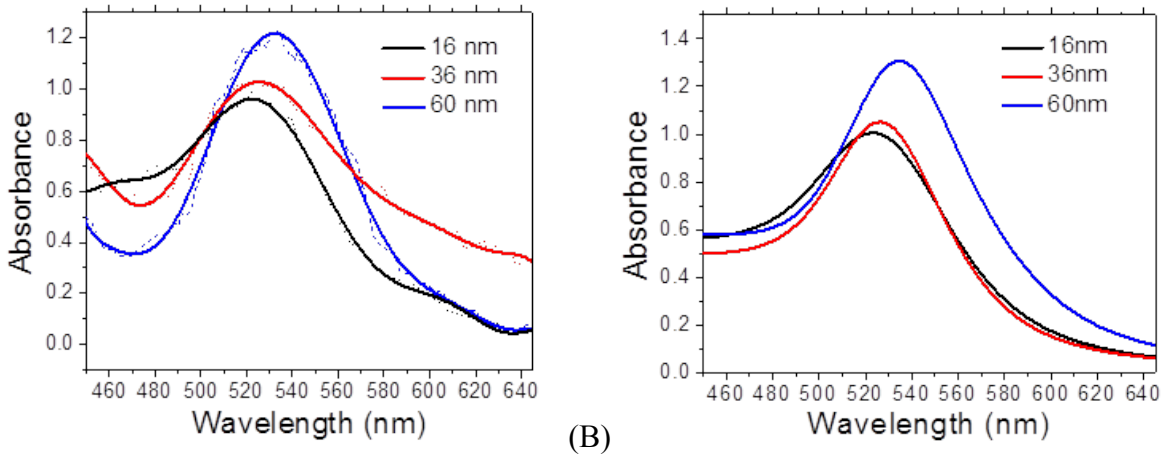
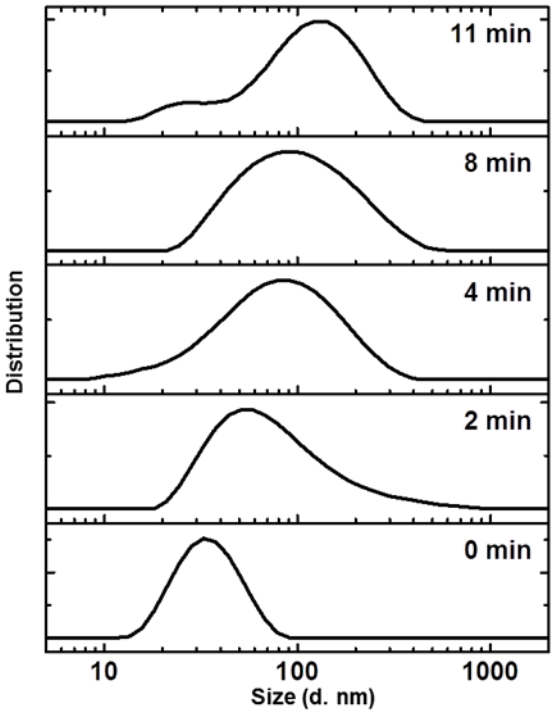
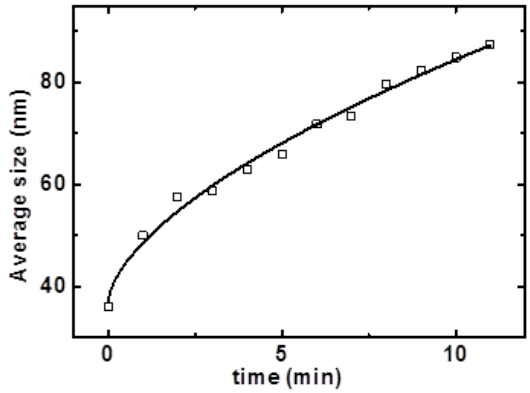


Fig.S4 The absorbance spectra of gold nanoparticles with diameter of 16, 36 and 60 nm were measured by (A) smartphone spectrometer and (B) UV/Vis spectrometer. The spectra in (A) were fitted by polynomial with an order of 9.

Fig. S5 shows the dynamic light scattering (DLS) measurement on the peptide-functionalized AuNPs (36 nm) after the incubation of 100 ng/ml cTnI. The average size of AuNPs increases from 36 nm up to 90 nm after 10 min incubation of cTnI, due to the cTnI induced aggregation of AuNPs.



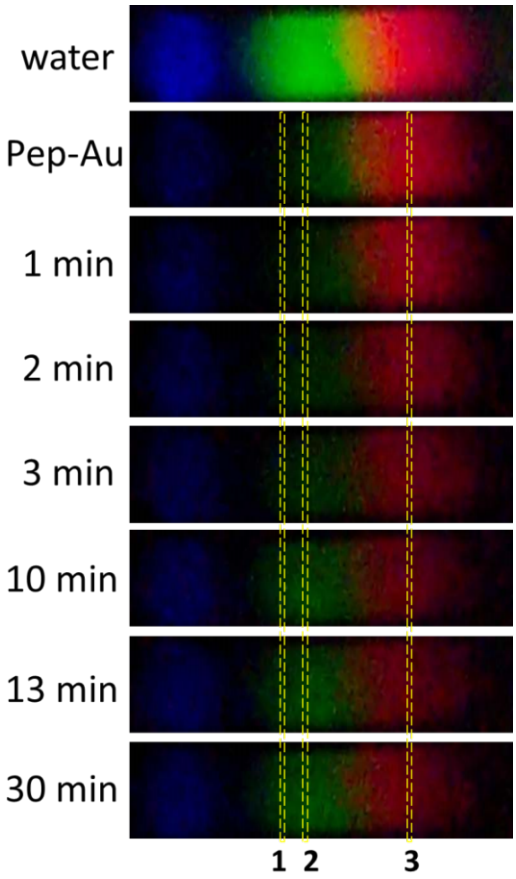
(A)



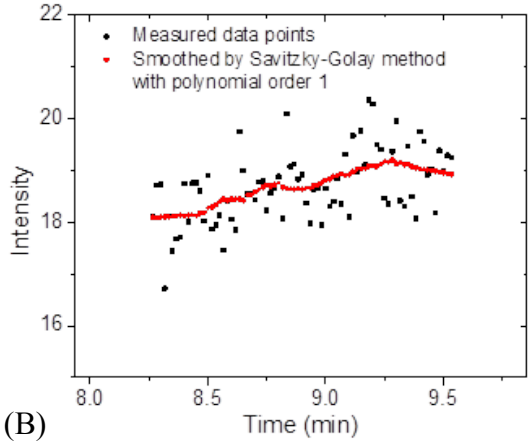
(B)

Fig. S5 (A) The DLS data of peptide-functionalized AuNPs (36 nm) upon incubation with 100 ng/ml cTnI for 0 to 11 min. (B) The time-dependent average size changes of AuNPs obtained from the DLS measurement.

Fig. S6 shows the "rainbow" band changes of peptide-functionalized AuNPs after incubation with cTnI, as measured by smartphone spectrometer. The intensity changes on the color band at position 1, 2, 3 were monitored in real-time. To decrease the noise level on the time-dependent intensity changes, the measured data points were smoothed by Savitzky-Golay method with 20 points of window and polynomial order of 1, as an example shown in Fig. S6B. The kinetics can be further plotted with exponential fit (Fig. S6C). The noise level obtained from the smoothed data was 3 times of the standard deviation measured on AuNPs, σ=3×SD (Fig. S6D). The detection limit of about 50 ng/ml was estimated as the concentration of cTnI at which the response is equal to the noise level.



(A)



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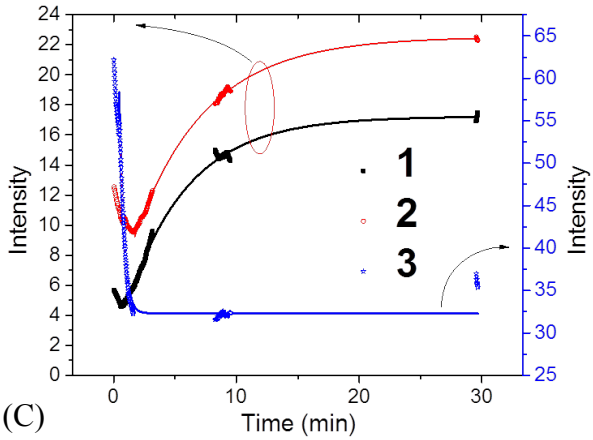

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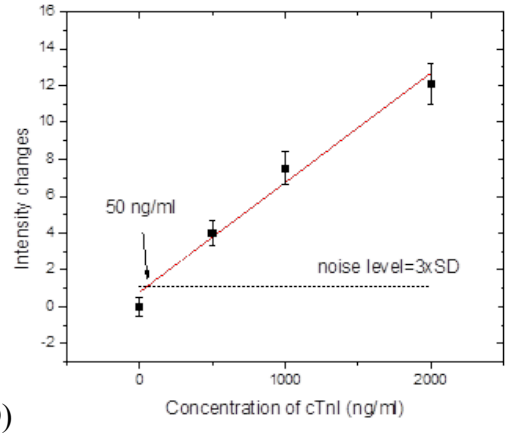
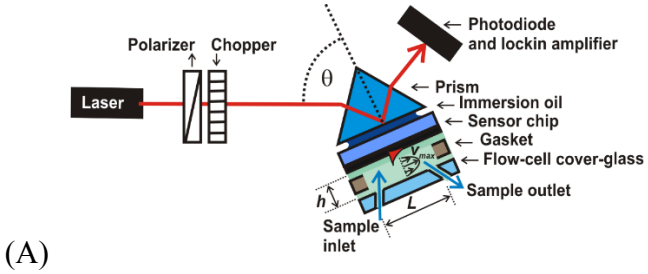


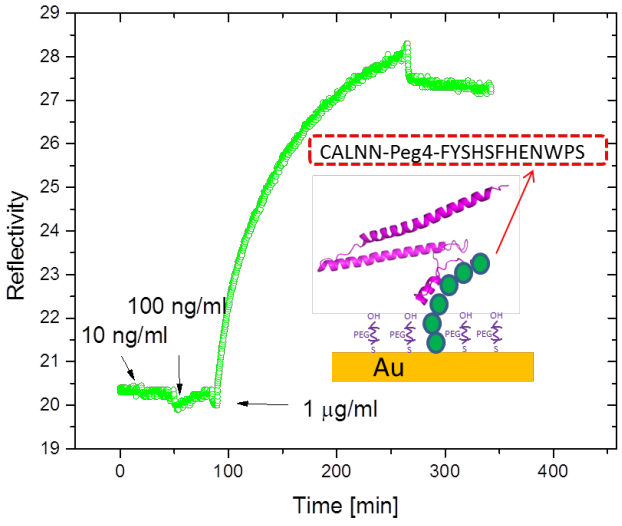
(D)

Fig. S6 (A) The color bands of water and peptide-functionalized AuNPs before and after incubation of 2μg/ml cTnI for 1 min to 30 min. (B) An example of time-dependent intensity obtained from smartphone spectrometer (at location 2 in A at during 8.5 to 9.5 min incubation with cTnI) and data smoothed by Savitzky-Gloay method with 20 points of window and polynomial order of 1. (C) The corresponding intensity changes (smoothed by Savitzky-Gloay) at location 1, 2, 3 (corresponding to wavelength of about 525 nm, 540 nm and 615 nm, respectively) in A indicating the molecular binding process. (C) The calibration curve for the detection of cTnI in PBS buffer, as measured by smartphone spectrometer. The intensity changes were obtained at wavelength of 540-542 nm.

The SPR measurement was carried out on a home-built setup as indicated in one of our published paper (Fig.S7A).[1] A glass chip coated with 2 nm Cr and 47 nm Au was modified with peptide and Thiol-PEG at molar ratio 1:1. The binding affinity was monitored by the reflectivity changes upon the injection of cTnI to the senor chip.



(A)



(B)

Fig. S7 (A) A scheme of the SPR setup. (B) SPR reflectivity measurement of peptide-functionalized gold film on the incubation of cTnI at concentration of 10 ng/ml, 100 ng/ml and 1 μg/ml.

The XNano instrument (Insplorion, Sweden) was employed to measure the absorbance spectra and peak wavelength changes of peptide-functionalized AuNPs upon the incubation of cTnI at concentration from 10 ng/ml to 1 µg/ml. The absorbance peak increases from 525 nm up to 535 nm in 5-min incubation of cTnI. As the low noise level (σ=3×SD=0.0455 nm), it shows lower detection limit down to 15 ng/ml as compared with our smartphone spectrometer. However, the sensitivity of this AuNPs-based colorimetric assay can be further improved by optimization the peptide affinity, surface chemistry and particles sizes.

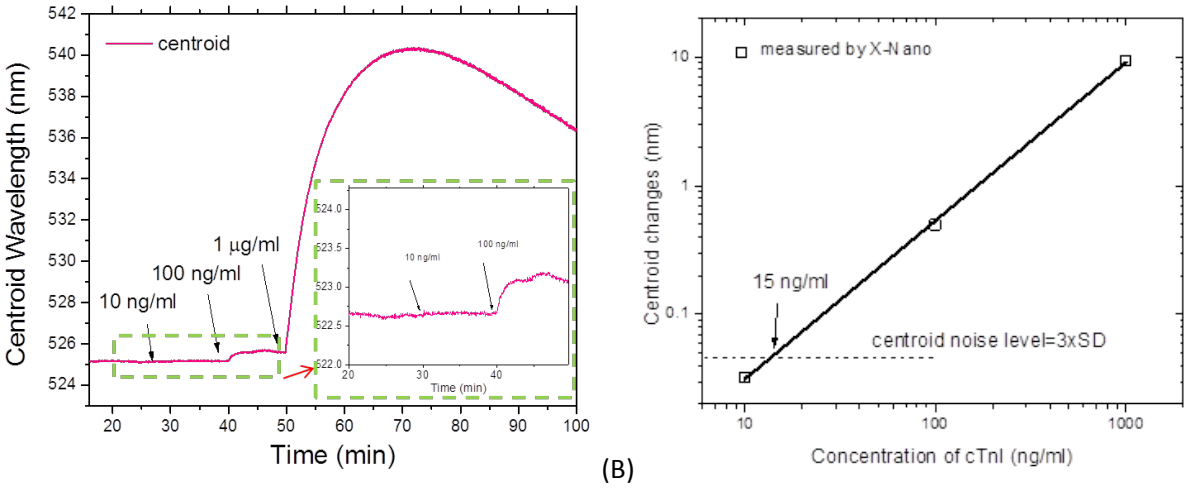


Fig. S8 (A) The time-dependent centroid wavelength (corresponding to absorbance peak) of peptide-functionalized AuNPs upon the addition of cTnI at final concentration of 10 ng/ml, 100 ng/ml and 1 µg/ml, measured on Insplorion XNano (Insplorion, Sweden). (B) The centroid changes at 5 min after addition of cTnI as function of the concentration of cTnI. It indicates the detection limit of about 15 ng/ml.

References

1. Wang, Y.; Huang, C.-J.; Jonas, U.; Wei, T.; Dostalek, J.; Knoll, W. Biosensor based on hydrogel optical waveguide spectroscopy. *Biosensors and Bioelectronics* **2010,** *25*, 1663-1668.