Determination of Nanoparticles by UV-Vis Spectra

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(a)



(b)



(c)



(d)



(e)



(f)



(g)



(h)



(i)



(j)



(k)



(l)

Figure S1: (a-l) Absorbance spectrums of various pigments, with their chemical structures, before and after exposure to the different NPs (at various concentrations) at pH of 7.41.





Figure S2: Results of the PCoA analysis on 7 different types of nanoparticles at 6 concentrations (i.e. 10, 20, 40, 60, 80, and 100 ng/ml)



Figure S3: Results of the HCA on 7 different types of nanoparticles at 6 concentrations (i.e. 10, 20, 40, 60, 80, and 100 ng/ml)

Synthesis of Gold Nanoparticles

Various gold nanoparticles (*i.e.*, gold nanospheres (NS20; ~20 nm), gold nanospheres (NS30; ~30 nm), short gold nanorods (NR4; aspect ratio of 4), and long gold nanorods (NR20; aspect ratio of 20)) were synthesized according to the previous report.¹

Preparing of chromophore solutions. Chromophore solutions were prepared in PBS with a maximum visible absorbance of 1.0 (concentrations were in order of 1.0×10^{-5} to 1.0×10^{-6} M). The pH of solutions was fixed with HCl and NaOH at 7.41. The absorbance measurements were done after one minute of exposure with NPs. Since the polarity of the solvent effect on the absorption spectrum⁷, only the water solvent was used to prepare solutions.

Results of the synthetic NPs.

Aqueous solutions of all indicators were prepared in phosphate buffered saline (PBS), with peak absorbance 1.0 before the addition of the NPs. Figure S5 shows the initial normalized absorbance of the dye solutions, covering the visible range from 380 to 750 nm. Various gold NPs (*i.e.*, spheres with various sizes (20 and 30nm), short rod, and long rod) were characterized by TEM and UV/vis spectroscopy approaches (see Figure S4). It is notable that none of NPs showed the plasmonic absorption peak at concentrations lower than 1ppm.



Figure S4. UV-Vis absorbance of (a) Au nanospheres and (b) Au nanorods (AR \sim 4); (c–f) transmission electron microscopy images of gold nanospheres (NS20; \sim 20 nm), gold nanospheres (NS30; \sim 30 nm), short gold nanorods (NR4; aspect ratio of 4), and long gold nanorods (NR20; aspect ratio of 20), respectively. Reproduced with permission from reference 1.



Figure S5. Normalized absorbance overlay of selected indicators in water (at pH of 7.41).

Each type of the employed gold NPs, at various concentrations (i.e., 10, 25, 50, 100, 250, 500, 1000, 2500, and 5000 ng/ml) was exposed to various indicator solutions and the spectra of solutions were recorded after one minute (see Figure S6). The spectral changes of indicators after interaction with gold NPs provide a facile and rapid way for identification of NPs. Spectral changes for all indicators produce a specific pattern for each NP at different concentrations. As can be seen from Figure S6, responses of various dyes to the existence of different NPs are not similar.



(a)

















(g)



Figure S6. Absorbance spectrums of various dyes (a-h) before and after exposure to the different NPs (A-D; at various concentrations) at pH of 7.41.

A color difference map, which is a useful approach for visualization of the achieved data was performed by subtraction of the light absorbance before and after exposure between 3 selected visible wavelengths (*i.e.* 558, 590 and 616 nm). As shown in Figures 5, the resulting color difference pattern provides a robust fingerprint for each NPs at different concentrations. According to the maps, one can easily distinguish the type of NPs without need to any statistical technique. Color change profiles for four different gold NPs as a function of concentration are also in Figure 6. The colorimetric sensor array has also been tested against interference of Au^{3+} , CTAB and pH changes (range of 0.1), as a control cases. In this case, no responses were observed in the selected wavelengths. The values of limits of detection (LOD) and limit of quantification (LOQ), based on the colorimetric maps, were presented in Table S1.



Figure S7. Color difference maps for various nanoparticles and 4 controls.



Figure S8. Color difference maps of nanoparticles (at different concentration) and 4 control done in triplicate.

Table S1. The value of LOD and LOQ for the nanoparticles according to the results of color difference maps.

	NR ₂₀	NR_4	NS_{20}	NS ₃₀
LOR(ng/mL)	10	25	250	250
LOQ(ng/mL)	<10	10	10	10







(b)



(c)



380

480

580

. 680







Congo Red Omin 3min 6min

9min 9min 12min 15min











(e)











(h)

Figure S9. Absorbance spectrums of various dyes (a-h) before and after exposure to the different NPs (at 5μ g/mL concentrations) at pH of 7.41. A) Long rod B) Short rod C) Sphere20nm, and D) Sphere30nm

References

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