Supporting information for the paper:

# Hemoprotein bioconjugates of Au and Ag nanoparticles and Au nanorods: structure-function correlations

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## Supporting Information 1

### Calculation of coverage

We illustrate the calculation with the example of Hb.

(a) Cross sectional area of Hb molecule, circle with diameter 5.5 nm $= \pi r^2$

$= 3.14 \times (2.75\ nm)^2$

$= 23.75\ nm^2$

(b) Cross sectional area of Hb molecule ellipse with diameters 5.5 nm and 7 nm $= \pi r_1 r_2$

$= 3.14 \times (2.75\ nm \times 3.5\ nm) = 30.22\ nm^2$

Average cross sectional area from (a) and (b) $= 27\ nm^2$

In order to get the layer thickness of an adsorbed layer, we calculate the average diameter of the molecule. This is necessary as the adsorption can occur the horizontal or perpendicular direction (note that the molecule is an ellipsoid).

Average diameter of the molecule = [5.5+5.5+7.0]/3 nm = 6 nm

Surface area of Ag nanoparticle with diameter 60 nm $= 4\pi r^2$

$= 4 \times 3.14 \times (30\ nm)^2$

$= 11304\ nm^2$

Maximum coverage on first layer = 11304 $nm^2$ / 27 $nm^2$

= 419

Surface area of second layer on Ag nanoparticle (d= [6 + 60 + 6] nm) = $4\pi r^2$

= 4 X 3.14 X $(36\ nm)^2$

= 16277.76 $nm^2$

Maximum coverage on second layer = 16277.76 $nm^2$ / 27 $nm^2$

= 603

Similarly, the number of molecules in the 3rd, 4th and 5th layes can be calculated as, 821, 1072 and 1357, respectively.

Therefore, the number of molecules in 4 layers of Hb on Ag (60 nm) particle

= 419 + 603 + 821 + 1072

= 2915

The experimentally observed figure namely, 2858 is close to the calculated one and the difference can be due to reduced packing density.

## Supporting Information 2

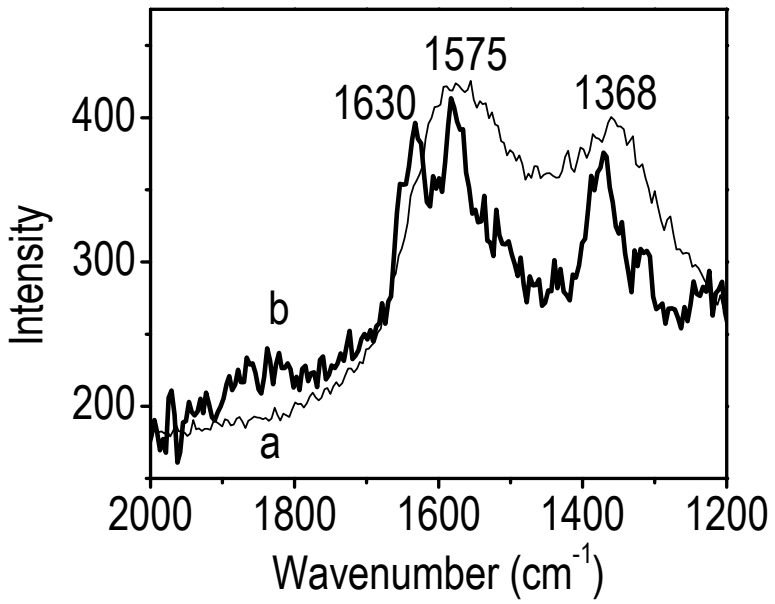


**Figure 1.** Raman spectra of Mb (a) and AuNR@Mb (b), recorded using 514.5 nm laser excitation through a confocal (60 X) objective.

## Supporting Information 3

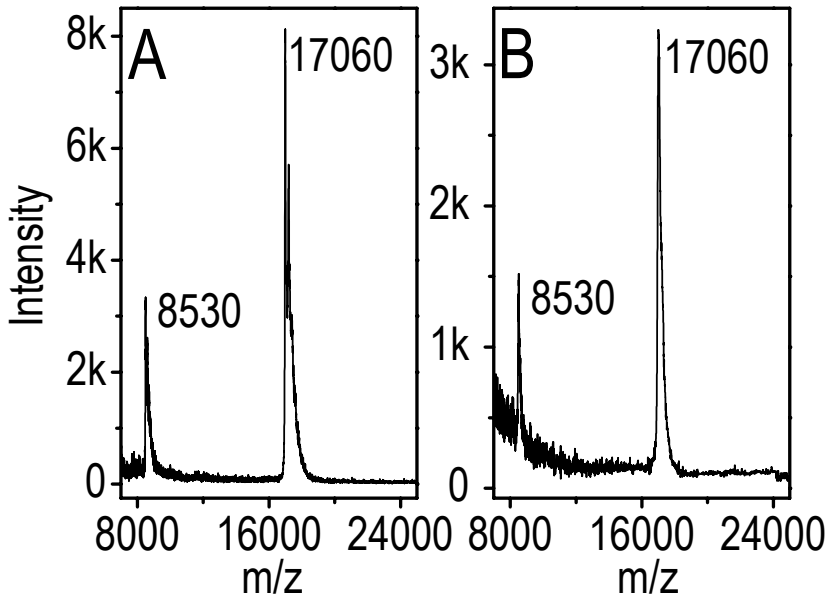


**Figure 2.** MALDI –TOF mass spectra of the samples measured with 337 nm $N_2$ laser using sinapinic acid matrix. The figures A and B correspond to Mb and AuNR@Mb, respectively.

## Supporting Information 4

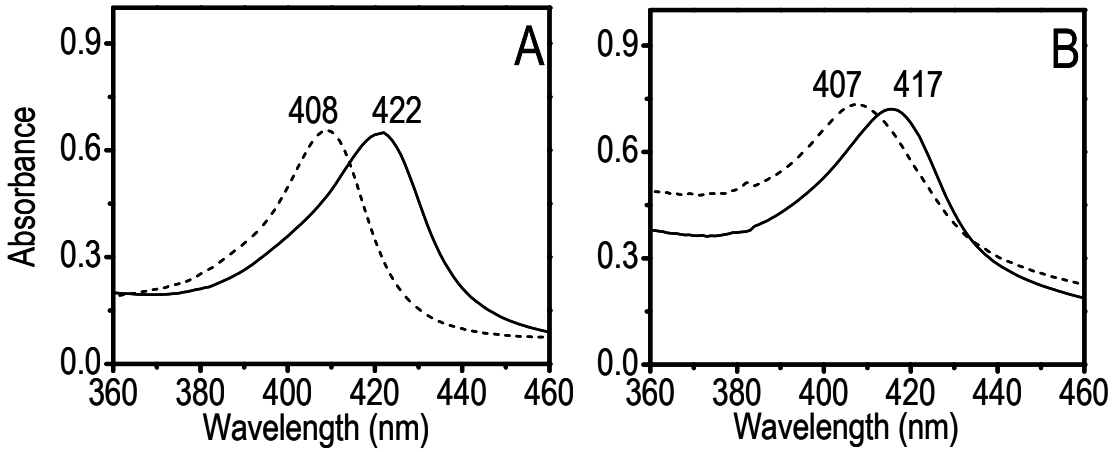


**Figure 3.** Absorption spectra of Mb (A) and Hb (B) in aqueous phosphate buffered saline. The solid line and dashed lines correspond to samples kept with 10 mM sodium azide for 24 hours and control sample without sodium azide, respectively.

**Supporting Information 5**

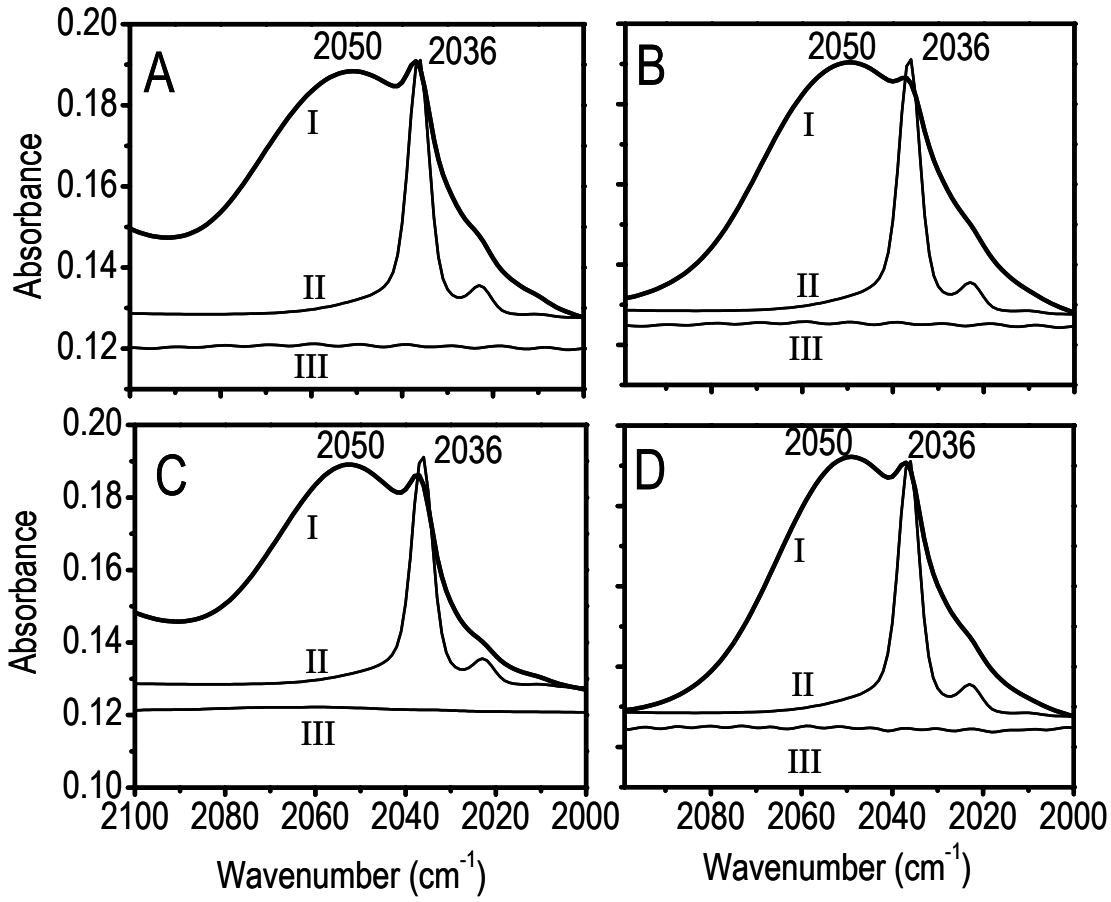


**Figure 4.** FTIR spectra of Au@Mb-$N_3$ (A), Ag@Mb-$N_3$ (B), Au@Hb-$N_3$ (C) and Ag@Hb-$N_3$ (D) recorded in KBr matrix. Traces (I), (II) and (III) of A, B, C and D represent M@X-$N_3$, M@$N_3$ and M@X, respectively.

## Supporting Information 6

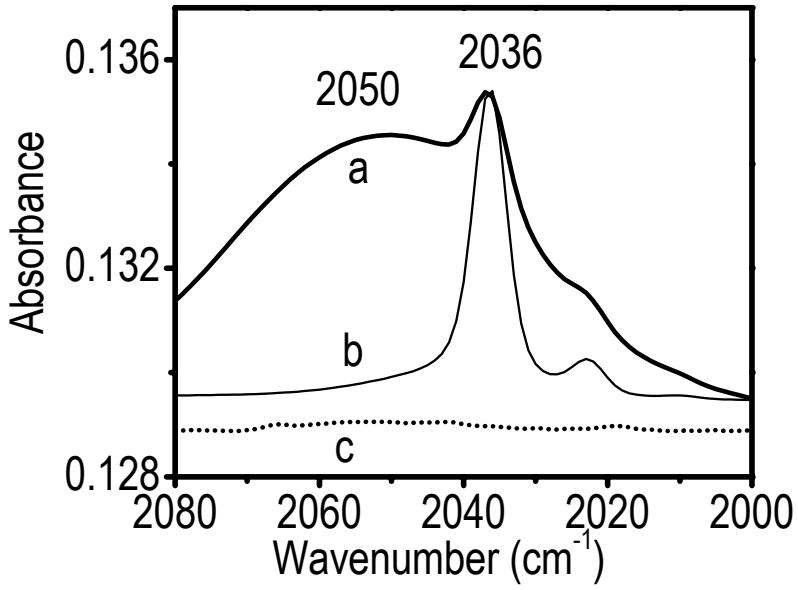


**Figure 5.** FTIR spectra recorded in KBr matrix. Traces (a), (b) and (c) represent AuNR@Mb-$N_3$, AuNR@$N_3$ and AuNR@Mb, respectively.