Supplementary Information

A photochemically initiated chemistry for coupling underivatized carbohydrates to gold nanoparticles
Xin Wang, a Olof Ramström, *a,b Mingdi Yan *a

a Department of Chemistry, Portland State University, P.O. Box 751, Portland, Oregon, 97207-0751;
b Department of Chemistry, KTH - Royal Institute of Technology, Teknikringen 30, S-10044 Stockholm, Sweden

1. Mannose density measurement

Figure 1S. Calibration curve obtained by treating various concentrations of d-mannose with anthrone/sulfuric acid and measuring the absorption at 620 nm.
2. Characterization of PFPA-functionalized and mannobiose-conjugated Au NPs

Figure 2S. $^1$H NMR spectra of PFPA-disulfide 1 and gold nanoparticles functionalized with PFPA-disulfide 1 (Au-PFPA) in CDCl$_3$ with TMS ($\delta$ 0.0 ppm).
Figure 3S. FT-IR spectra of PFPA-disulfide 1, gold nanoparticles functionalized with PFPA-disulfide 1 (Au-PFPA), and Au NPs subsequently coupled with α-1,4-mannobiose (Au-DiMan). The azide (-N$_3$) absorption at ~2125 cm$^{-1}$ disappeared after light activation.
3. Calculation of D-mannose density on Au NP

![D-mannose molecule and Au NP](image)

Figure 4S. D- mannose molecules and Au NPs

The maximal number of D-mannose molecules on each Au NP is calculated as follows.

Assuming that D-mannose occupies in space by taking the shape of a square, each side of the square is measured to be ~ 6Å by Chem 3D (CambridgeSoft., Ultra, version 9.0).

The D-mannose molecule is then projected to the surface, and the surface area of each D-mannose molecule is 36 Å².

The surface area of one 20-nm Au NP is $1.26 \times 10^5$ Å² ($= 4\pi \times 100^2$).

The maximal number of D-mannose molecules occupying the surface of one Au NP in a closely packed manner is $3.50 \times 10^3$ ($=1.26 \times 10^5$ Å²/36 Å²), corresponding to $5.81 \times 10^{-12}$ nmol [$=3.50 \times 10^3/(6.02 \times 10^{23}) \times 10^9$].

Assuming that the density of Au NPs equals to that of gold (19.3 g/cm³), the weight of each 20-nm Au NP is $8.08 \times 10^{-14}$ mg ($=19.3 \times (4/3 \pi \times 10^3) \times 10^{-21} \times 10^3$).

The number of Au NPs in 1 mg of Au NPs is $1.24 \times 10^{13}$ ($=1/8.08 \times 10^{-14}$), which is equivalent to 0.0206 nmol ($=1.24 \times 10^{13} / (6.02 \times 10^{23}) \times 10^9$).

The theoretical maximal amount (mole) of D-mannose on 1 mg Au NP is 72.0 nmol ($=5.81 \times 10^{-12} \times (1.24 \times 10^{13})$).

The D-mannose density of Au NP coated was measured to $24.1 \pm 1.7$ nmol/mg Au NPs. Therefore, the number of D-mannose molecules on each 20-nm Au NP is ~$1.17 \times 10^3$ ($=24.1/0.0206$).

The surface coverage, ie measured/theoretical, is 33.4% ($=1.17 \times 10^3 /(3.50 \times 10^3)$).
4. Control experiments

Figure 5S. UV-vis spectra of PFPA-functionalized Au NPs and after treating with 100 nM and 1000 nM Con A.