Supporting Information

Design of oligoaziridine-PEG coatings for efficient nanogold cellular biotagging

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Estimation of the number of ligands per gold nanoparticle

According to TEM images and DLS measurements (Figure 2 and Table 1), the average diameter of the nanoparticles is 28 nm. Assuming the spherical shape for the particles, the volume of each particle is $(4/3)\pi(d/2)^3 = 1.15\text{x}10^{-17}$ cm^3. Hence the mass of each particle (M_{au}) is ($19.3\text{x}10^3$ mg/cm^3) x ($1.15\text{x}10^{-17}$ cm^3) = $2.22\text{x}10^{-13}$ mg. From TGA analysis of MPM coated AuNP (Figure S1A) the amount of gold core is 1.4 mg. So the number of gold nanoparticles (N_{Au}) is ($1.4 / 2.22\text{x}10^{-13}$) = $6.31\text{x}10^{12}$. Also, from the TGA data, the amount of MPM (M_w= 3400 g/mol) present is 0.10005 mg. Therefore, the number of MPM molecules (N_{MPM}) is ($0.100\text{x}10^{-3}$) x ($6.023\text{x}10^{23}$) / 3400 = $1.77\text{x}10^{16}$ and the number of MPM molecules per one AuNP is N_{MPM}/N_{Au} = 2807.

From TGA analysis of OA coated AuNP (Figure S1B) the amount of gold core is 2.63 mg. So the number of gold nanoparticles (N_{Au}) is ($2.63 / 2.22\text{x}10^{-13}$) = $1.19\text{x}10^{13}$. Also, from the TGA data, the amount of OA (M_w= 997.50g/mol) present is 0.10005 mg. Therefore, the number of OA molecules (N_{OA}) is ($0.171\text{x}10^{-3}$) x ($6.023\text{x}10^{23}$) / 997.5 = $1.03\text{x}10^{17}$ and the number of OA molecules per one AuNP is N_{OA}/N_{Au} = 8712.

In order to understand how much OA and MPM are grafted onto particles' surface in the sample Au-MPM-OA, an ICP analysis for the sulfur atom was performed. Considering that each mol of S origins 1 mol of OA, the amount of OA/AuNP (grams) is $9.63\text{x}10^{-3}$. Therefore, considering the amount of gold core (1.6 – (0.04 x 1.6)) = 1.536 mg, the amount of OA is ($1.54\text{x}10^{-3}$) x ($9.63\text{x}10^{-3}$) = $1.48\text{x}10^{-5}$ g. Hence the mass of MPM in the weight loss from Au-MPM-OA (0.064 mg), is ($1.6 - 1.536 - 1.48\text{x}10^{-5}$) = $6.40\text{x}10^{-5}$g. Therefore, the number of molecules of OA would be ($1.48\text{x}10^{-5}$) x $6.023\text{x}10^{23}$ / 997.50 = $8.93\text{x}10^{15}$ (results obtained from TGA analysis Figure S1C). Consequently, the number of molecules of MPM is ($6.40\text{x}10^{-5}$) x $6.023\text{x}10^{23}$/ 3400 = $1.13\text{x}10^{16}$. Since the number of gold nanoparticles (N_{Au}) is ($1.536 / 2.22\text{x}10^{-13}$) = $6.93\text{x}10^{12}$, the number of molecules of MPM per one AuNP is 1636 as the number of molecules of OA per one AuNP is 1289. Thus, the total number of molecules per one nanoparticle is 2925.

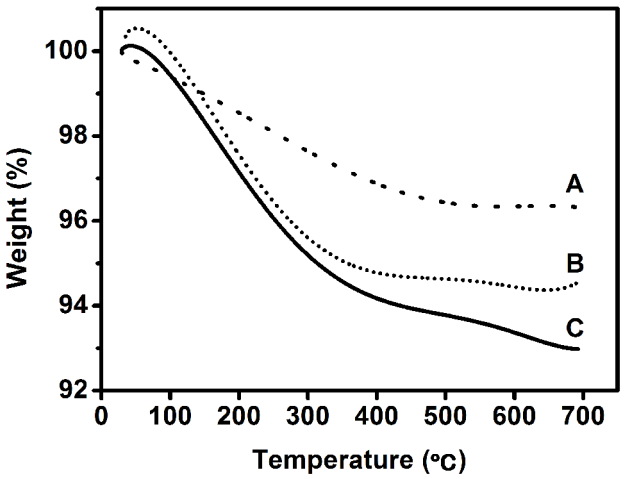

Figure ESI 1. TGA curves of A) Au-MPM, B) Au-OA and C) Au-MPM-OA nanoparticles. .

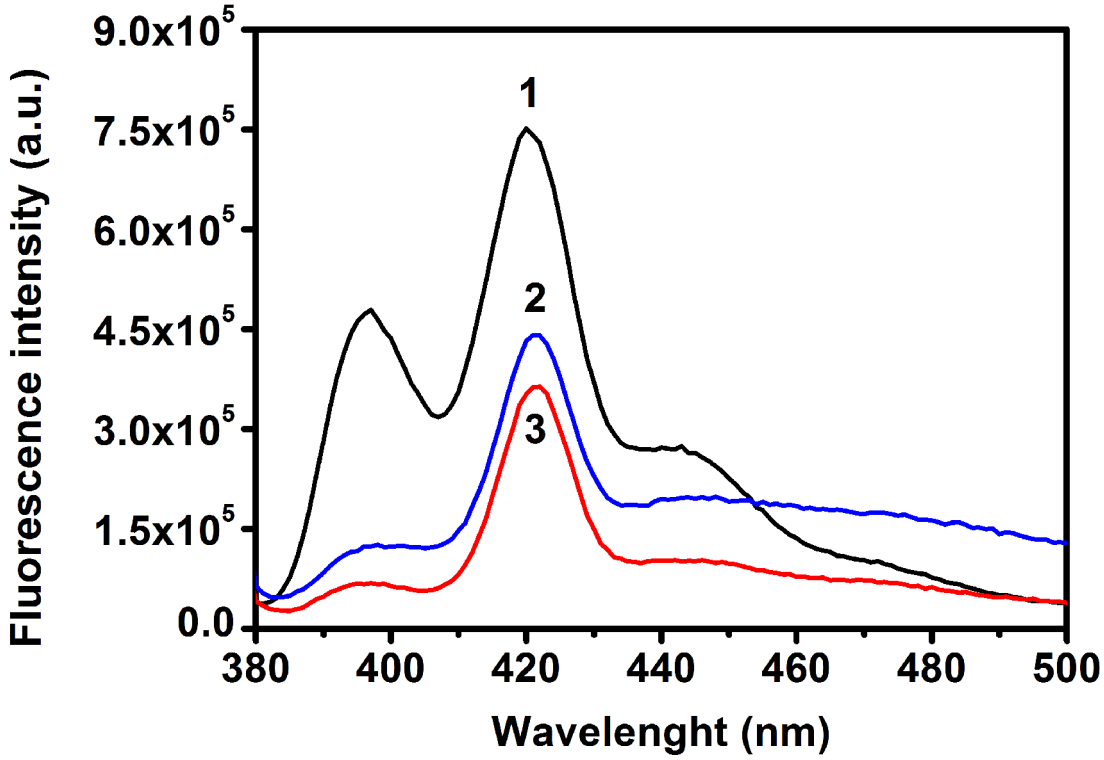

Figure ESI 2. Fluorescence spectra of 1) OA, 2) Au-OA and 3) Au-MPM-OA biosensors.

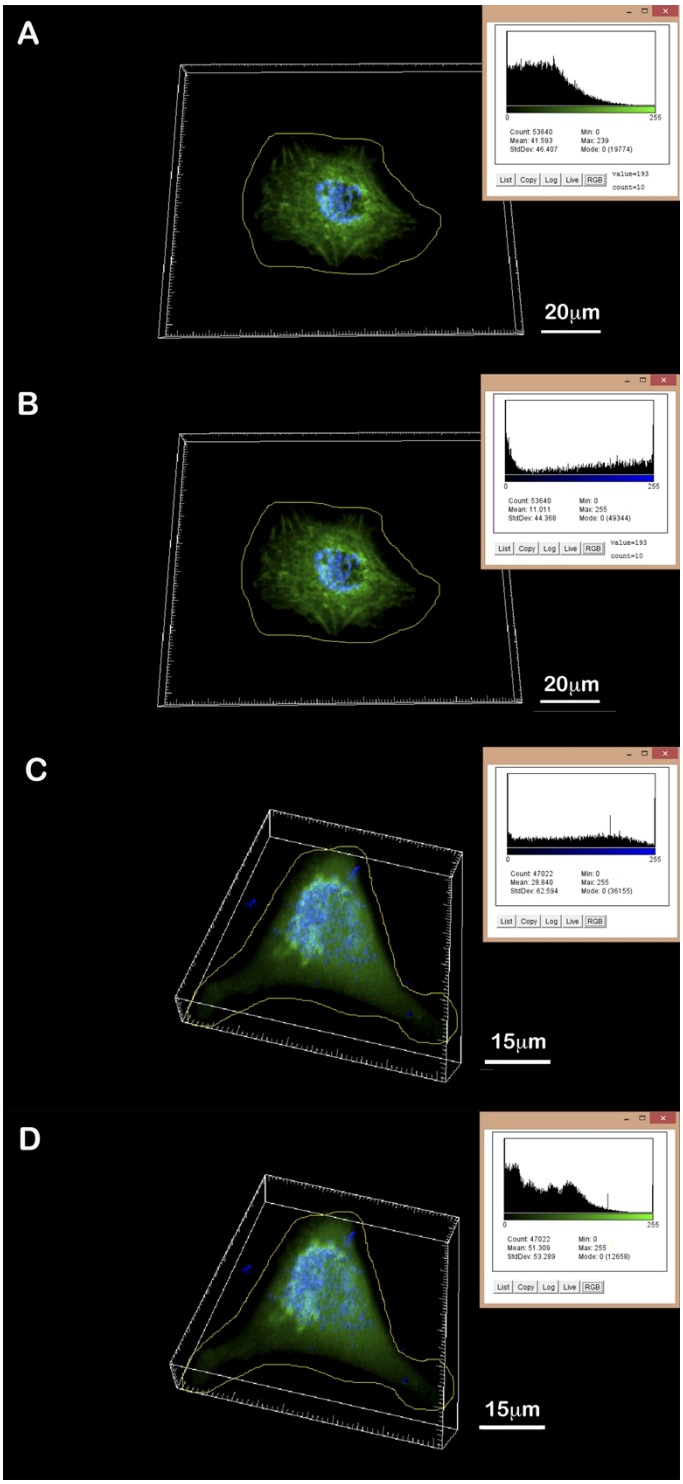

Figure ESI 3. Image J color histograms: A) CLSM images of A549 cells transfected with Au-OA, green histogram; B) CLSM images of A549 cells transfected with Au-OA, blue histogram; C) CLSM images of A549 cells transfected with Au-MPM-OA, green histogram; CLSM images of A549 cells transfected with Au-MPM-OA, blue histogram. Green color – CellLight® Actin-GFP, BacMam 2.0; Blue color – GNP; Yellow color – region of interest selection.

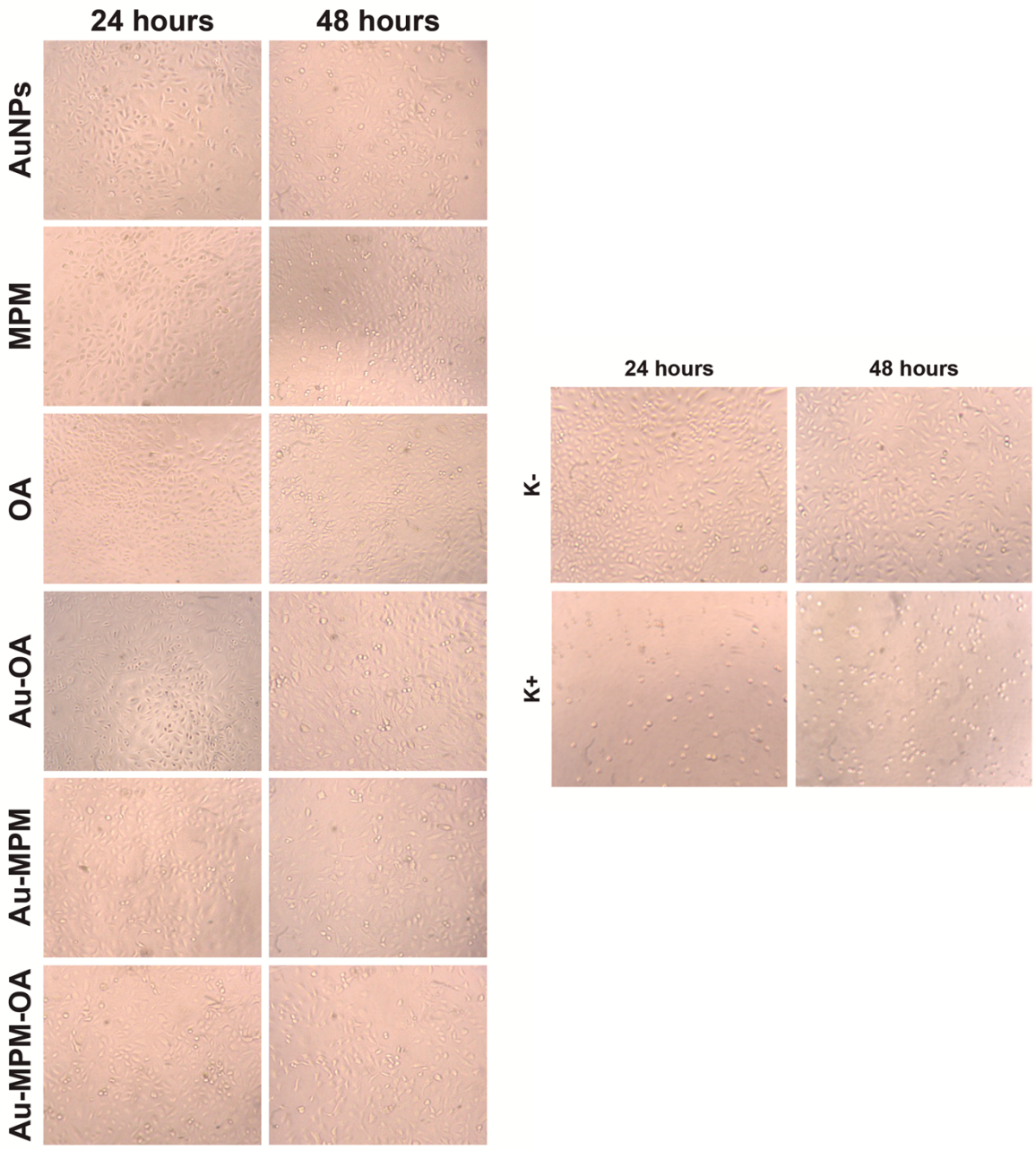

Figure ESI 4. Optical micrographs of A549 cell line transfected with the produced biotags and respective precursors after 24 h and 48 h of incubation: Gold nanoparticles (AuNPs); Maleimide-PEG-Maleimide (MPM); Oligoaziridine Biosensor (OA); Gold nanoparticles coated with oligoaziridine (Au-OA); Gold nanoparticles capped with Maleimide-PEG-Maleimide (Au-MPM); Gold nanoparticles capped with Maleimide-PEG-Maleimide and oligoaziridine (Au-MPM-OA); Negative control (K-) and Positive control (K+). Original magnification x 100.