SUPPORTING MATERIALS FOR:

Upconverting organic dye doped core-shell nano-composites for dual-modality NIR imaging and photo-thermal therapy

Guobin Shan, Ralph Weissleder, and Scott A. Hilderbrand*

*Corresponding author

Center for Systems Biology, Massachusetts General Hospital and Harvard Medical School, 185 Cambridge St, CPZN 5210, Boston, MA 02114. Tel. 617-643-5679 Email Scott_Hilderbrand@hms.harvard.edu

Figure S1: Structure of CyTE-777 triethoxysilane.

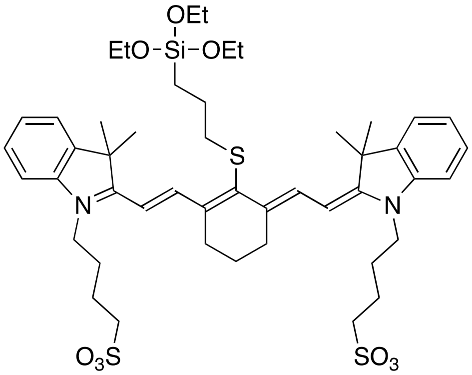


Figure S2: Low resolution negative ion electrospray mass spectrogram of the crude ethanolic reaction solution containing CyTE-777 triethoxysilane.

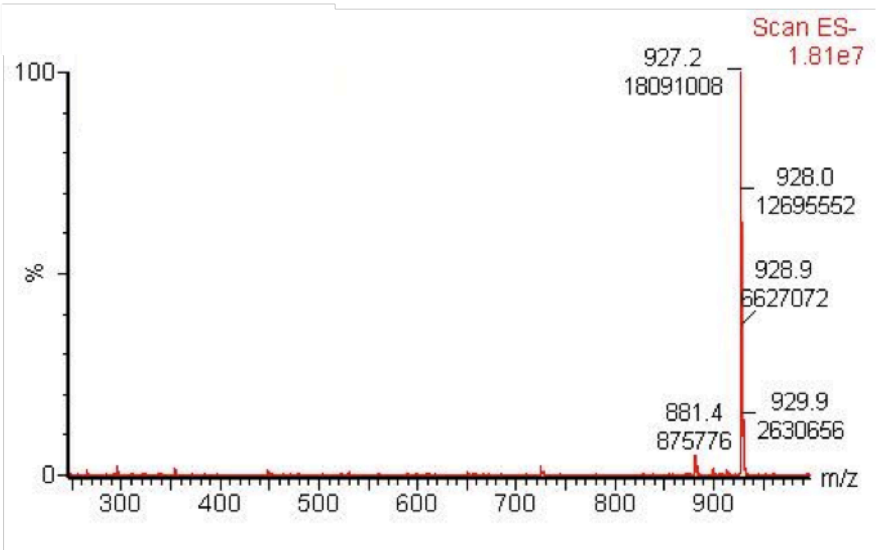


Figure S3: Absorbance spectra and corresponding fluorescence spectra of absorbance matched aqueous solutions of IR783 and UNP@SiO$_2$/Dye nano-composites under identical conditions

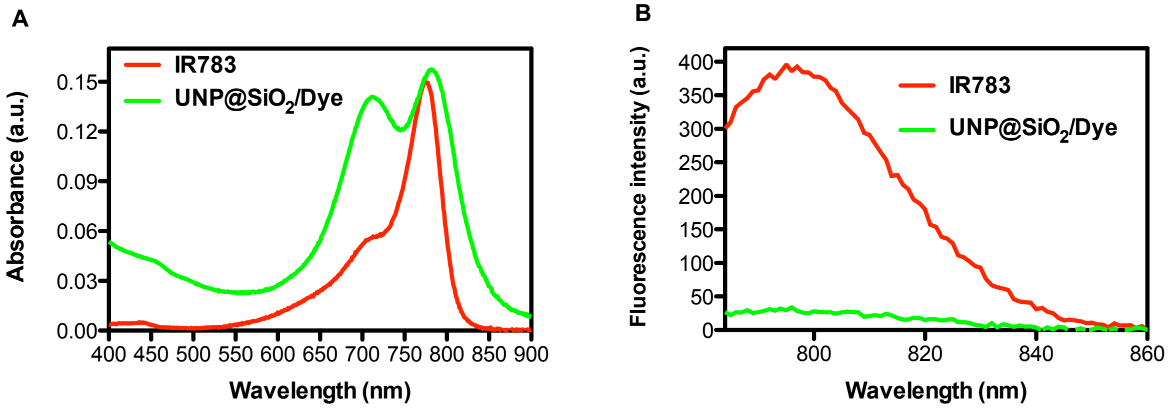


Figure S4: (a) Molar absorbance coefficients (ε, M^{-1}cm^{-1}) for the UNP@SiO$_2$/Dye nano-composite and gold nanorods; and (b) mass absorption coefficients (ε, mL·mg^{-1}cm^{-1}) for the UNP@SiO$_2$/Dye nano-composite and gold nanorods. All measurements are in water.

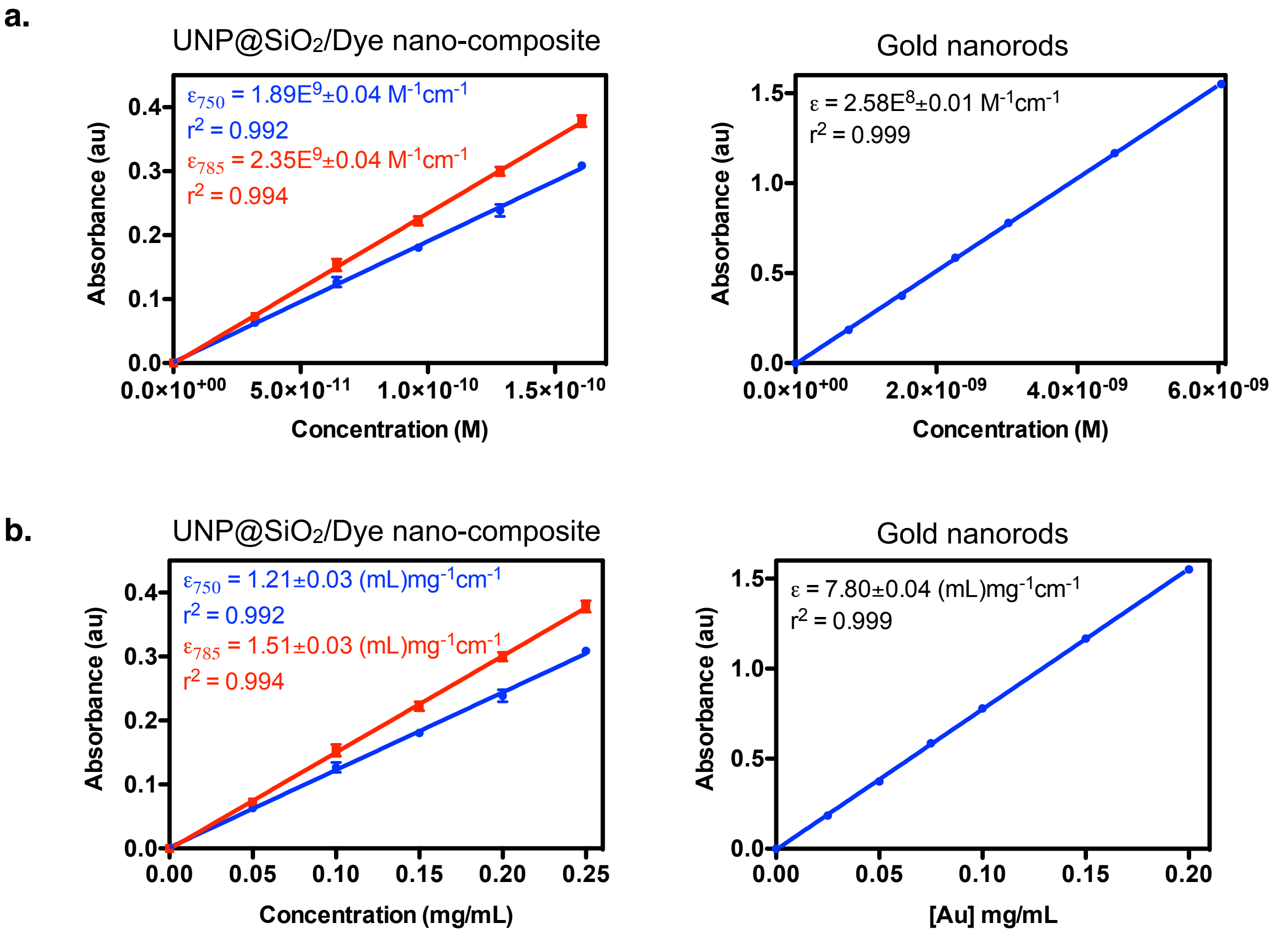


Figure S5: Stability of UNP@SiO_2/Dye nano-composites in water.

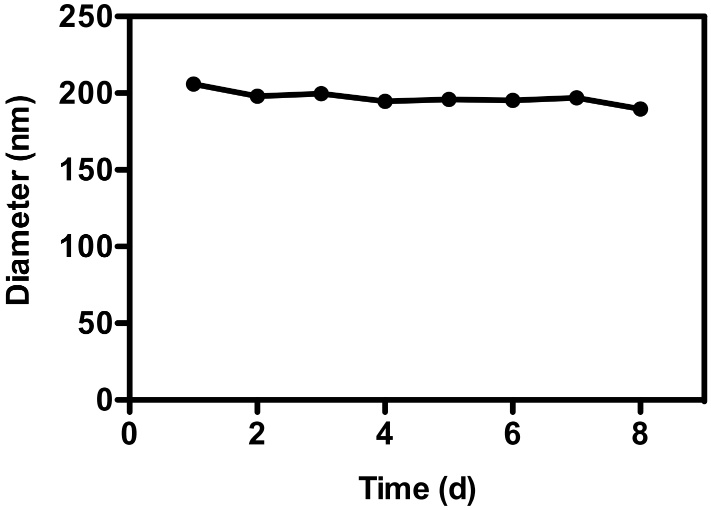


Figure S6: X-ray diffraction pattern of the UNP core.

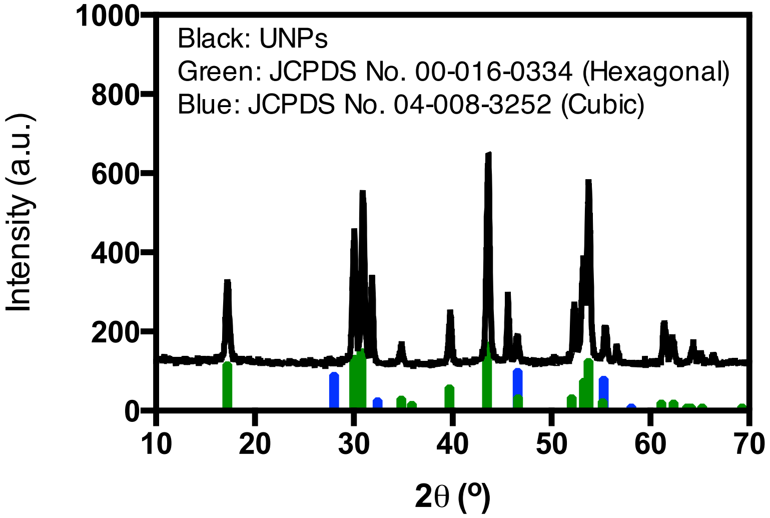
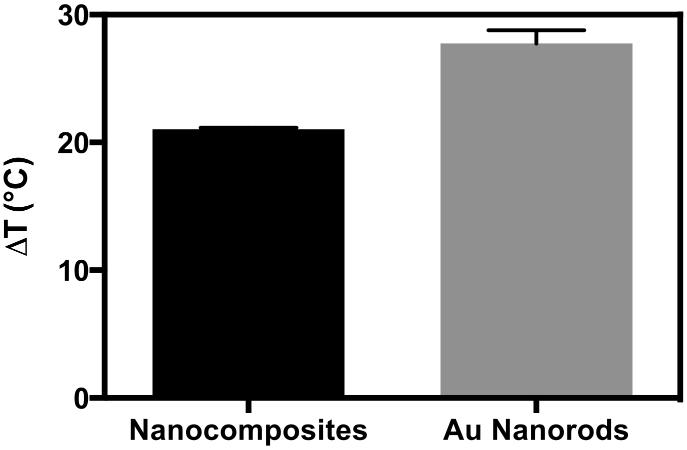


Figure S7: Delta Temperature (120 seconds) of 2.0 mg/mL nano-composites and 2.0 mg/mL gold (Au) nanorods (purchased from NANOCS Inc). These Au nanorods exhibit plasmonic absorption at 750 nm.



Heating efficiency calculations

The heating efficiencies for the UNP@SiO_2/Dye nano-composite and Au nanorod samples under excitation at 750 nm in our experimental setup were estimated based on the heat capacity of water and the Beer-Lambert Law.

1) Energy consumption for water heating ($\mathbf{W_{water}}$, *J*):

$$\mathbf{W_{water} = m \cdot C_w \cdot \Delta T}$$

where **m** is the mass of water, (g); $\mathbf{C_w}$ is the heat capacity of water, (4.18 $J \cdot g^{-1} \cdot K^{-1}$) and $\mathbf{\Delta T}$ is the change in temperature of the water (deg. K).

2) Energy input from light absorbance ($\mathbf{W_{input}}$, *J*):

$$\mathbf{W_{input} = (I_o - I) \cdot t}$$

where $\mathbf{I_o}$ is the intensity of light before entering the solution (W); **I** is the intensity of light after passing through the solution (W); and **t** is the exposure time (s).

According to the Beer-Lambert Law,

$$\mathbf{I/I_o = 10^{-\varepsilon lc}}$$

Solving for **I**,

$$\mathbf{I = I_o \cdot (10^{-\varepsilon lc})}$$

where $\boldsymbol{\varepsilon}$ is the mass absorbtivity, ($mL \cdot mg^{-1} \cdot cm^{-1}$); **l** is the distance the light travels through the solution in *(cm)*; and **c** is the concentration of the nanoparticles in solution ($mg \cdot mL^{-1}$).

Therefore combining the above equations,

$$\mathbf{W_{input} = \{I_o - I_o \cdot (10^{-\varepsilon lc})\} \cdot t}$$

3) Heating efficiency of nanoparticle ($\boldsymbol{\eta}$, *%*)

$$\eta = W_{water}/W_{input} \times 100$$

In these experiments:

$\mathbf{m}$ = 0.025 g

$\mathbf{C_w}$ = 4.18 $J \cdot g^{-1} \cdot K^{-1}$

$\Delta \mathbf{T_{nanocomposite}}$ = 21 K

$\Delta \mathbf{T_{Au}}$ = 27 K

$\mathbf{I_o}$ = 0.15 W

$\mathbf{t}$ = 120 s

$\boldsymbol{\varepsilon}_{\mathbf{nanocomposite}}$ = 1.21 $mL \cdot mg^{-1} \cdot cm^{-1}$

$\boldsymbol{\varepsilon}_{\mathbf{Au}}$ = 7.80 $mL \cdot mg^{-1} \cdot cm^{-1}$

$\mathbf{l}$ = 0.04 cm

$\mathbf{c}$ = 2.0 mg/mL

Notes: Unless otherwise stated, all experimental values are the same for the nano-composite and Au nanorod heating experiments. Mass absorptivity coefficients (ε, $mL \cdot mg^{-1} \cdot cm^{-1}$) at 750 nm for the UNP@$SiO_2$/Dye nano-composite and Au nanorods were calculated via serial dilution according to Beers Law, see Fig. S4

From the above data and relationships, it follows that the heating efficiencies for the **UNP@SiO_2/Dye nanocomposite** ($\eta_{nano\text{-}composite}$) and **Au nanorod** ($\eta_{Au}$) samples are approximately **14 %** and **16%**, respectively. These heating efficiency values include energy loss to the surroundings (air, sample chamber, etc.) in our experimental setup.