Supporting information for:

Preparation of fluorescent Au-SiO_2 core-shell nanoparticles and nanorods with tunable silica shell thickness and surface modification for immunotargeting

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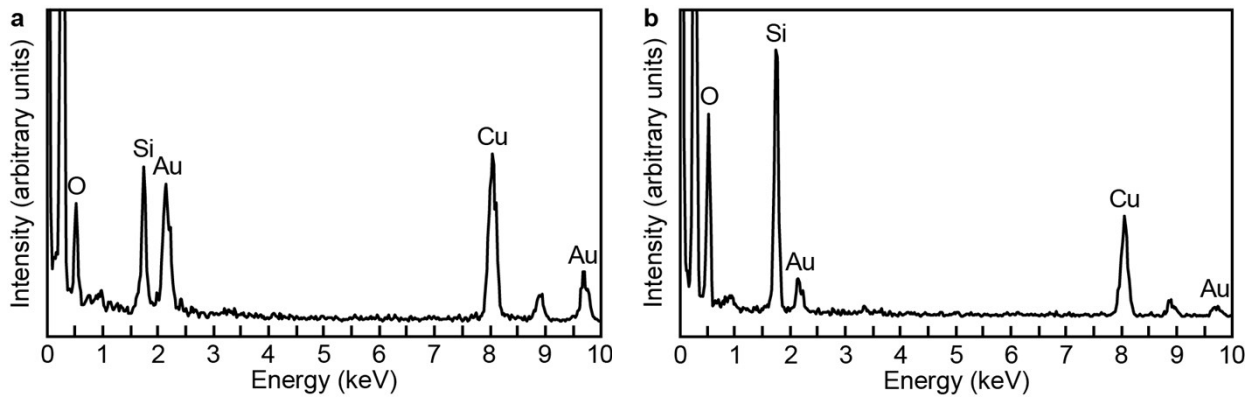


Fig. S1. EDS spectra for core-shell Au NPs prepared by the (a) modified Stöber method and (b) reverse microemulsion method. The presence of Au and Si was verified by the Au M_α emission at 2.120 keV and the Si K_α emission at 1.739 keV. Differences in the relative intensity of Si and Au peaks reflected a greater silica shell thickness from the reverse microemulsion method.

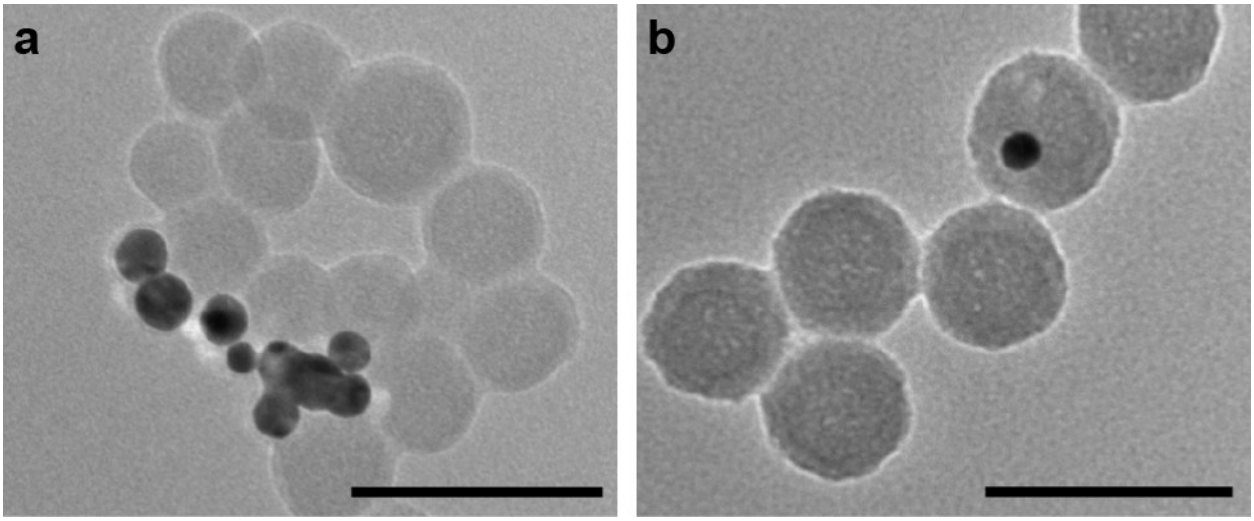


Fig. S2. Representative TEM micrographs of Au-SiO_2 core-shell NPs prepared by the reverse microemulsion method with (a) 11 mM and (b) 2.26 mM Au-oleylNH_2 NPs, showing the importance of optimizing the concentration of the Au-oleylNH_2 NPs for 1:1 incorporation of the Au NP core and silica shell. Scale bars = 100 nm.

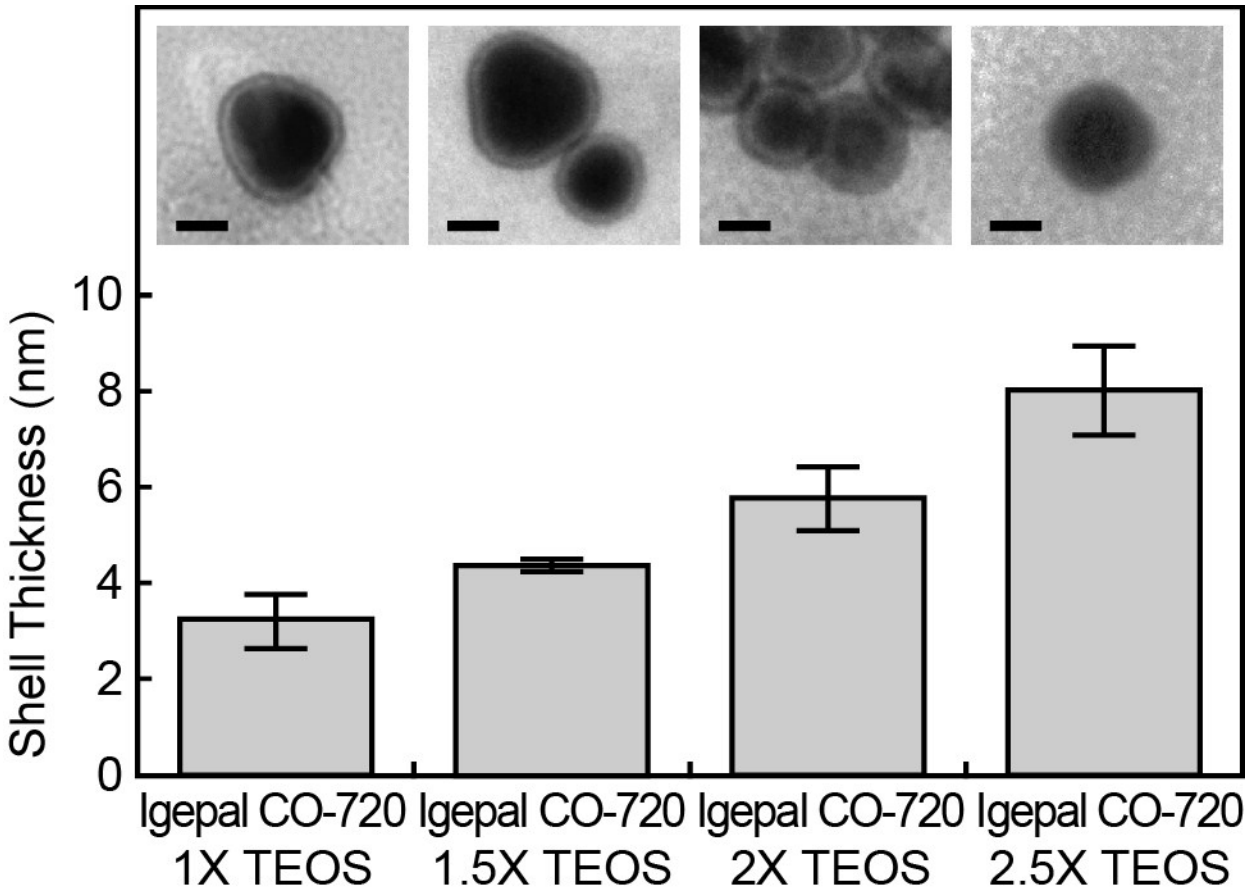
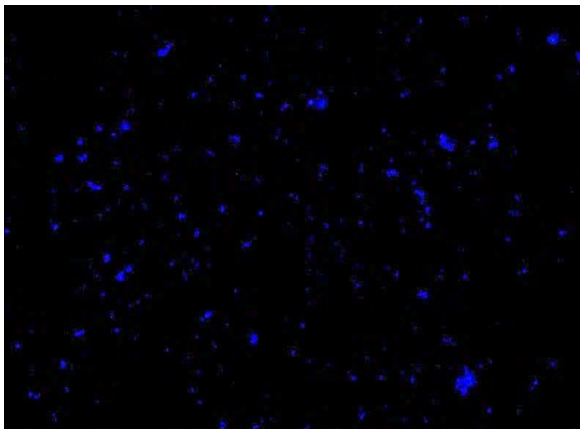
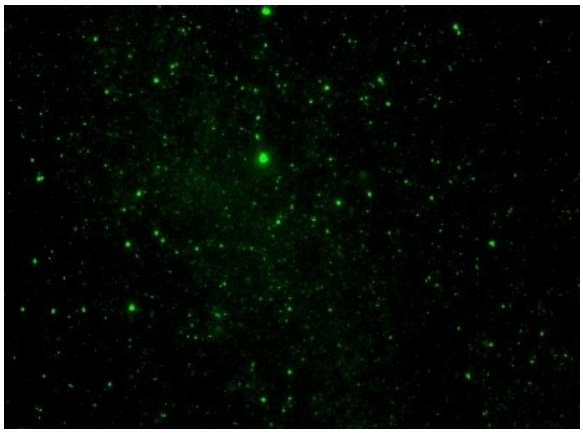


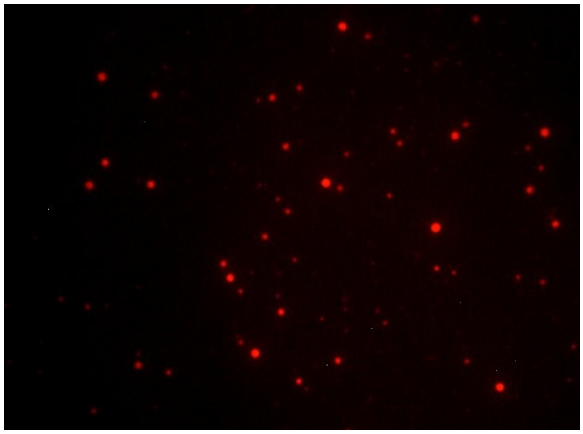
Fig. S3. Representative TEM micrographs showing the effects of the TEOS concentration on the measured silica shell thickness of cuboidal Au-SiO_2 NPs prepared by the reverse microemulsion method. The Au core and silica shell are visibly darker and lighter, respectively, due to the greater electron density of Au. Scale bars = 20 nm. Error bars show standard deviation of the mean. The mean ± standard deviation of silica shell thickness from left to right was 3.2 ± 0.6, 4.4 ± 0.1, 5.7 ± 0.7 and 8.0 ± 0.9 nm. Note that the concentration of Igepal CO-720 was held constant at 0.2 M for each preparation and 1X TEOS corresponded to 22.5 mM TEOS. Also, note that the cuboidal Au NPs cores were prepared by the same conditions used for Au NRs (Fig. 5) except that 1 mM $AgNO_3$ was used instead of 4 mM $AgNO_3$. Additionally, the CTAB capping agent was ligand exchanged with oleylamine in cyclohexane to yield cuboidal Au-oleylNH_2 NPs.



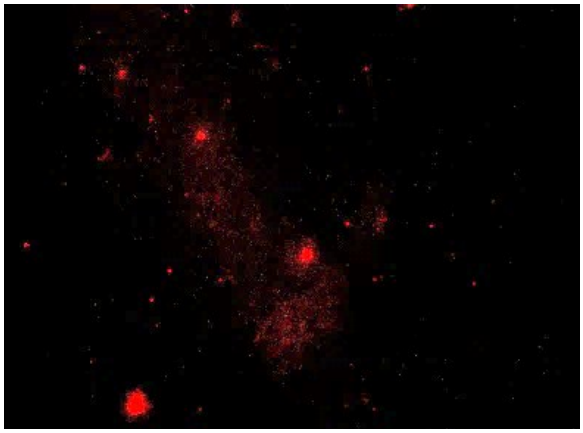
DyLight™ 350
ex/em = 353/432
874 g/mole



FITC
ex/em = 490/525
389 g/mole



RITC
ex/em = 543/580
536 g/mole



DyLight™ 594
ex/em = 593/618
1078 g/mole

Fig. S4. Epifluorescence micrographs showing the fluorescence emission from Au-SiO_2 core-shell NPs volume-labeled with DyLight™ 350 (blue), FITC (green), RITC (red), and DyLight™ 594 (red). The excitation/emission wavelength and molecular weight is listed for each fluorophore.

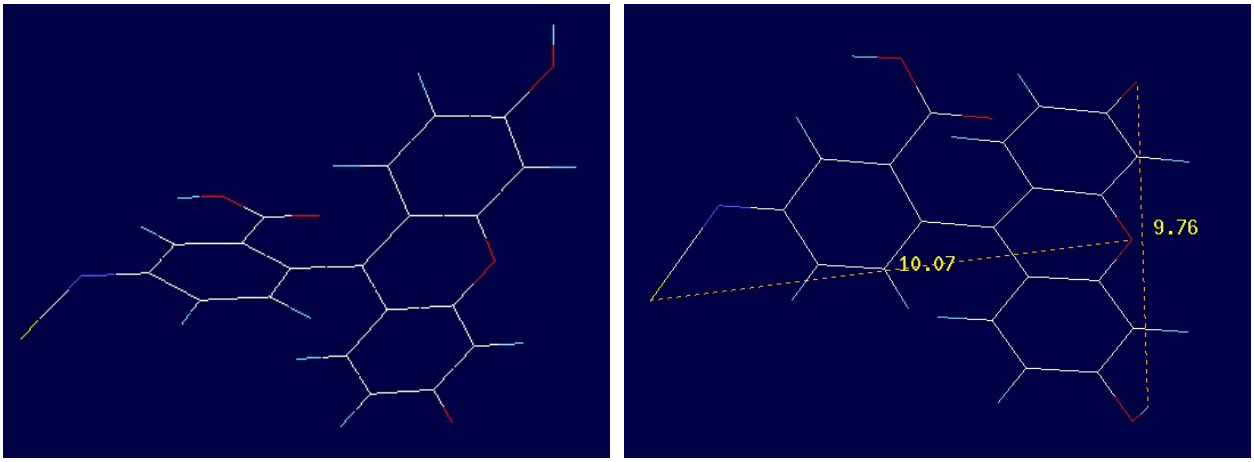


Fig. S5. Three-dimensional rendered Protein Data Bank (PDB, http://www.rcsb.org/pdb/, H. M. Berman *et al*., *Nucl. Acids Res*., 2000, **28**, 235) structure file of FITC showing an overall height of 10.07 Å, a width of 9.76 Å, and a maximum (square) footprint of 101.4 $Å^2$ (1.014 nm^2). A core-shell NP with a core 16 nm in diameter and a shell 10 nm thickness possesses a surface area of $4.07 \cdot 10^5$ $Å^3$ ($4.07 \cdot 10^3$ nm^3). Therefore, ~1700 to 2100 fluorophores can be tagged onto the surface of the silica shell assuming a binding efficiency of 40-50% (Pierce Chemicals)

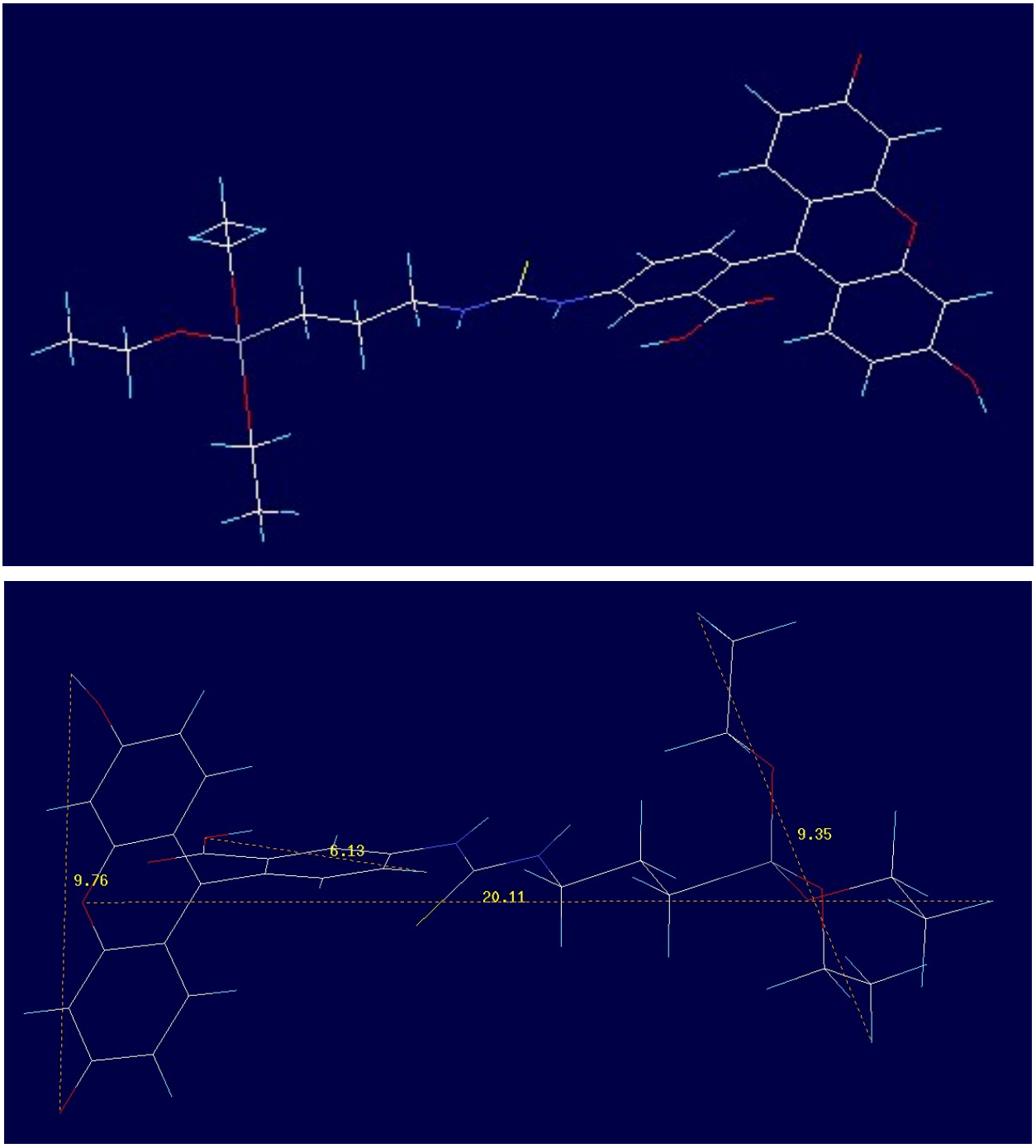


Fig. S6. Three-dimensional rendered PDB structure file of FITC-APTES, the fluorescent precursor volume-loaded into the silica shell of core-shell NPs in this study, showing an overall height of 20.11 Å, a width of 9.76 Å, a depth of 6.13 Å, and a maximum constraining volume of 1203.2 $Å^3$ (1.203 nm^3). A core-shell NP with a core 16 nm in diameter and a shell 10 nm thickness possesses a shell volume of $0.022 \cdot 10^9$ $Å^3$ ($0.022 \cdot 10^6$ nm^3). Therefore, up to ~18,500 fluorophores can be packed into the silica shell assuming dense packing.

Table S1. Theoretical comparison of fluorophore loading in core-shell NPs using covalent linking to the shell surface versus encapsulation within the shell volume showing the greater number of fluorophores that can be loaded onto a single core-shell NPs by volume-loading.

Silica shell thicknesses (nm)	Number of FITC molecules conjugated to the silica shell surface, *X* *	Number of FITC molecules encapsulated in the silica shell volume, *Y*	Ratio of volume encapsulated to surface conjugated FITC molecules, *Y*/*X*
1	502	756	1.5
2.3	657	2023	3.1
2.5	683	2249	3.3
3.5	819	3514	4.3
2.4	670	2135	3.2
2.6	696	2365	3.4
3.8	863	3940	4.6
4	892	4236	4.7
10	2008	18531	9.2
14	2999	35306	11.8

*50% binding efficiency was assumed for isothiocyanate molecules (Pierce Chemicals).