Electronic Supplementary Information (ESI)

Decontamination of nanoparticles from aqueous samples using supramolecular gels

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Sr. No.		Content	
1	Material	rials and Methods	
	1.1	Materials	S2
	1.2	General procedure for hydrogel formation to entrap nanoparticles (QDs, lysine-capped AuNPs and TiO ₂ -NPs)	S2
2	Physicochemical Characterization		
	2.1	Fluorescence Spectroscopy	S3
	2.2	UV-Visible Spectroscopy	S3-S5
	2.3	Transmission Electron Microscopy (TEM) Experiments	S5-S7

Table of content

1. Materials and Methods

1.1 Materials

5'-(4-((2*H*,2*H*,3*H*,3*H*-perfluoroundecanamide)methyl)-1*H*-1,2,3-triazole-1-yl)*N*3-)1-((β-Dglucopyranoside)-1*H*-1,2,3-triazole-4-yl)methyl)thymidine was used as Glycosylated-Nucleoside Fluorinated amphiphiles (GNFs) for hydrogels formation. GNF,(Godeau et al., 2010) water soluble encapsulated quantum dots (QDs, size ≤ 20 nm, concentration = 17 µg/mL in water)(Aimé et al., 2013) and lysine-capped gold nanoparticles (AuNPs, size ≤ 20 nm, concentration = 10⁻⁴ M)(Selvakannan et al., 2003) were synthesized according to the literature procedure. Titanium oxide (Rutile) in water dispersion (5-30 nm APS, (15% TiO₂ by weight)) was purchased from Nanostructured and amorphous materials, Inc. (CAS No. #1317-80-2 and #7732-18-5). Working concentration of TiO₂ was 100 mg/L (0.001 M NaCl solution). Milli-Q[®] water was used throughout the experiments unless otherwise noted.

1.2 General procedure for hydrogel formation to entrap nanoparticles (QDs, lysinecapped AuNPs and TiO₂-NPs)

Hydrogel formation in the presence of nanoparticle solution (QDs, lysine-capped AuNPs and TiO₂-NPs) was actualized with very low concentration of GNF (0.1 % (w/v), i.e. 1.0 mg of GNF in 1.0 mL of nanoparticle solution). GNF powder and aqueous nanoparticle solution (QDs, lysine-capped AuNPs and TiO₂) were added to the micro tube/test tube. Hydrogels were prepared by heating this solution at 80 °C with constant shaking till it gave transparent solution (2 to 3 min.). Allow this solution to settle down for 24 to 48 h. After 24 to 48 h there was a gel formation with supernatant liquid left behind. The supernatant liquid was separated carefully from the gel and analyzed.

2. Physicochemical Characterization

2.1 Fluorescence Spectroscopy

Fluorescence spectra of functionalized QDs and supernatant liquid (after gel trapping experiments) were measured in a small-volume quartz cuvette and acquired using an LS 55 Perkin-Elmer instrument (xenon source excitation, FL WinLab software). Samples were excited at 350 nm (15 nm slit), and emission profiles were recorded from 555 to 655 nm (5 nm slit).

2.2 UV-Visible Spectroscopy

UV-Visible absorption spectra of lysine-capped gold nanoparticles (AuNPs) and Titanium dioxide nanoparticles (TiO₂-NPs) and respective supernatant liquid (after gel trapping experiments) were recorded on Carry 100 UV-Vis (Agilent Technologies) spectrophotometer.

2.2.1 Calibration Plot to calculate the concentration of GNF left behind in the supernatant liquid

The concentration of GNF left behind in the supernatant liquid (after hydrogel formation) was measured using UV-absorbance spectroscopy. To plot the calibration curve, seven different solutions having various amount of GNF were prepared and UV-visible absorbance spectra of these solutions were recorded (Fig. S1, Table S1). The concentrations of these solutions were selected in such a way that they gave homogeneous solution without forming a gel. The calibration graph (linear fit) for concentration vs. absorbance at 266 nm (λ_{max}) was plotted (Fig. S2). UV-visible absorbance spectra of supernatant liquid of GNF's hydrogel of three different concentrations were recorded (Fig. S3, Table S2) and the absorbance value (at 266 nm) was manipulated in the equation to calculate the amount of GNF left behind (Table S2). These experiments revealed that only 0.8-1.0 % of total GNF left behind in the supernatant liquid (Table S2).



Fig. S1 UV-visible absorbance spectra of GNF in DI water at different concentration

Sr. No.	GNF's concentration in mg/mL (X)	Absorbance at 266 nm (λ_{max}) (a.u) (Y)
01	0.01	0.04044823
02	0.025	0.13440205
03	0.05	0.29475829
04	0.1	0.57264209
05	0.2	1.19663763
06	0.3	1.70624769
07	0.4	2.27429414

Table S1 Absorbance value at 266 nm (λ_{max}) for GNF's solution at various concentrations



Fig. S2 Calibration plot for concentration of GNF (mg/mL) against absorbance (at 266 nm)



Fig. S3 UV-visible absorbance spectra of supernatant liquid of GNF-hydrogel in DI water at three different concentrations.

Sr. No.	GNF's concentration (mg/mL) (Z)	Absorbance of supernatant liquid at 266 nm (λ _{max}) (a.u) (Y)	Concentration of GNF left behind in the supernatant liquid (X) (mg/mL) through the following equation Y(Abs) = 5.7214 X (Conc.) + 0.0017	% of GNF left behind in the supernatant liquid = 100*X/Z
01	2	0.13105494	0.02260	1.13 %
02	5	0.25708231	0.04463	0.89 %
03	10	0.46506968	0.08098	0.81 %

Table S2 Absorbance value at 266 nm (λ_{max}) for supernatant liquid of GNF's hydrogel at various concentrations and concentration of GNF left behind in the supernatant liquid

2.3 Transmission Electron Microscopy (TEM) Experiments

TEM studies were performed on a HITACHI H7650 electron microscope in high resolution mode, at the BIC platform (Bordeaux Imaging Center). The software used for images acquisition was "Digital Micrograph (Gatan)". 10 μL of sample (GNF gel, lysine-capped AuNPs entrapped in GNF gel and TiO₂-NPs entrapped in GNF gel) were dispensed on a carbon-Formvar–coated 200-mesh nickel grid and dried for 10 min and stained with uranyl acetate just prior to observation.



Fig. S4 QDs entrapped in GNF's hydrogel (0.1 % (w/v)), TEM image (scale: 100 nm)



Fig. S5 Lysine-capped AuNPs with GNF (0.1 % (w/w)), TEM image (scale: 100 nm)