Electronic Supplementary Information (ESI)

Controlled DNA Condensation and Targeted Cellular Imaging by Ligand Exchange in Polysaccharide–Quantum Dots Conjugate

Yu-Hui Zhang, a Ying-Ming Zhang, a Yang Yang, a Li-Xia Chen a and Yu Liu* a,b

a Department of Chemistry, State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071 (P. R. China).

b Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300071 (P. R. China).

*Address correspondence to yuliu@nankai.edu.cn
**Experimental Section**

**General Methods.** All chemicals were reagent grade unless noted. The water-soluble HACD-coated QDs were prepared by the ligand exchange of trioctylphosphine oxide on the surface of pristine QDs with $\beta$-CD modified HA.\(^1\) ADA-AN\(^2\) were synthesized according to the reported methods. UV/Vis spectra were recorded in a conventional quartz cell (light path 10 mm) by using a Thermo Scientific EVOLUTION 300 spectrophotometer equipped with a HAAKE SC100 temperature controller to keep the temperature at 25 °C. Steady-state fluorescence emission spectra were recorded in a conventional quartz cell (10 × 10 × 45 mm) at 25 °C on a Varian Cary Eclipse equipped with a Varin Cary single-cell peltier accessory to control temperature. High-resolution transmission electron microscope (HR-TEM) images were obtained on a JEOL JEM-2010FEF high-resolution transmission electron microscope with an accelerating voltage of 200 kV. The samples were prepared by placing a drop of solution onto a carbon-coated copper grid and air-dried. AFM images were obtained on Veeco Nano IIIa Multimode atomic force microscope in tapping mode in air at room temperature. The sample solutions for DLS measurements were prepared by filtering the solution through a 0.45 μm filter into a clean cuvette. The zeta potential were recorded on NanoBrook 173Plus (Brookhaven company) at 25 °C. Gel electrophoresis was run on a 1% (w/v) agarose gel at 60 V for 30 min and photographed by means of a UV transilluminator and WD-9415B gel documentation system (Beijing Liuyi Instrument Factory, P. R. China). The fluorescent confocal images were carried out on a Leica TCS SP8 fluorescence microscope at $\lambda_{ex} = 405$ nm for DAPI, $\lambda_{ex} = 458$ nm for conjugate.
**Cytotoxicity Experiments.** NIH3T3 mouse embryonic fibroblast cell lines and MCF-7 human breast cancer cell lines were cultured in Dulbecco’s modified Eagle’s medium (DMEM), PC-3 human prostatic cancer cell lines were cultured in RPMI-1640 medium, both of the medium were supplemented with 10% fetal bovine serum (FBS). NIH3T3 cells, MCF-7 cells and PC-3 cells were seeded in 96-well plates (5 × 10^4 cells mL\(^{-1}\), 100 µL per well) for 24 h at 37 °C in 5% CO\(_2\). Then the cells were incubated with QDs–HACD, QDs–HACD/ADA-AN at different concentrations for 24 h and 48 h, respectively. The relative cellular viability was determined by the MTT assay. All data were presented as the mean ± standard deviation.

**Fluorescent Confocal Imaging.** NIH3T3 cells, MCF-7 cells and PC-3 cells were seeded in 6-well plates (5 × 10^4 cells mL\(^{-1}\), 2 mL per well) for 24 h at 37 °C in 5% CO\(_2\). The cells incubated with QDs–HACD/ADA-AN for 6 h, then the medium was removed, and the cells were washed with PBS for three times and fixed with 4% paraformaldehyde for 15 min. Then the cell nuclei were stained with DAPI (1 µg/mL) for 5 min. The cells were subjected to observation by a confocal laser scanning microscope.
Fig. S1 (a) UV-Vis spectrum and (b) fluorescence spectrum of QDs–HACD in aqueous solution. ([QDs] = 1 × 10^{-5} M, [HACD] = 1 × 10^{-4} M, \lambda_{ex} = 450 nm).
Fig. S2 (a) UV-Vis spectrum and (b) fluorescence spectrum of CdSe/ZnS QDs in hexane. ([QDs] = $1 \times 10^{-5}$ M, $\lambda_{ex} = 450$ nm).
Fig. S3 (a) The effect of HACD concentration on the FL intensity changes of QDs. (b) Langmuir binding isotherm description of the data showing a linear fitting over the HACD concentration range from 0.0091 to 0.18 mM. ([QDs] = 1.81 × 10^{-5} M, \lambda_{ex} = 450 \text{ nm}, I: \text{the fluorescence intensity of QDs–HACD})
**Fig. S4** Photographs of QDs–HACD conjugates at different QDs to HACD molar ratios of 1:1, 1:5, 1:10, 1:20 from left to right.

**Fig. S5** TEM images of QDs–HACD conjugates at ratios of (a) 1:0.5, (b) 1:1, (c) 1:5, and (d) 1:20.
**Fig. S6** Zeta potential of QDs–HACD conjugate at ratio of 10.

**Fig. S7** (a) AFM images, and DLS result of QDs–HACD/ADA-AN.
Fig. S8 AFM images of (a) pDNA, and (b) pDNA@QDs–HACD/ADA-AN.
Fig. S9 Relative cellular viability of PC-3 cell line: (a) 24 and (b) 48 h after the treatment with QDs–HACD, QDs–HACD/ADA-AN at different concentrations.
Fig. S10 Relative cellular viability of MCF-7 cell line: (a) 24 and (b) 48 h after the treatment with QDs–HACD, QDs–HACD/ADA-AN at different concentrations.
Fig. S11 Relative cellular viability of NIH3T3 cell line: (a) 24 and (b) 48 h after the treatment with QDs–HACD, QDs–HACD/ADA-AN at different concentrations.
**Fig. S12** Confocal fluorescence images of NIH-3T3 and MCF-7 cells incubated with pDNA@QDs–HACD/ADA-AN for 6 h. 4’,6-Diamidino-2-phenylindole dihydrochloride hydrate (DAPI) was used to stain nucleus.
References
