# Supporting Information

**Robust and Versatile Host-Guest Peptide Toolbox for Developing Highly Stable and Specific Quantum Dots-Based Peptide Probes for Imaging Extracellular Matrix and Cells**

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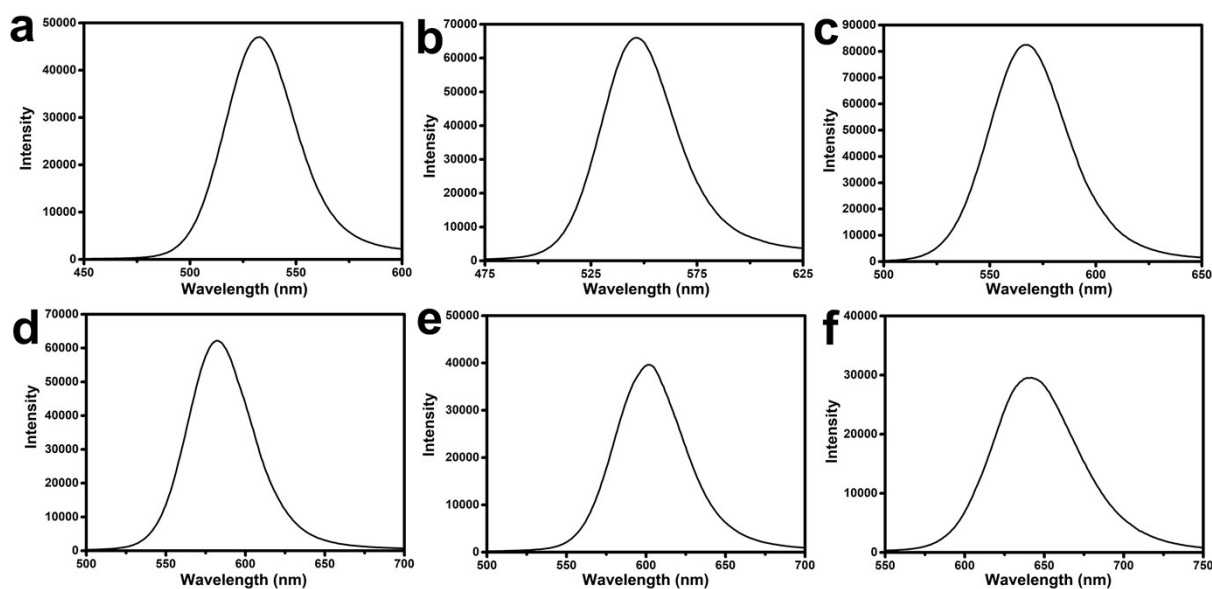
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**Fig. S1.** Fluorescence spectra of H1G1-QDs with maximum emission wavelengths of 530 nm (a), 545 nm (b), 565 nm (c), 585 nm (d), 605 nm (e) and 640 nm (f).
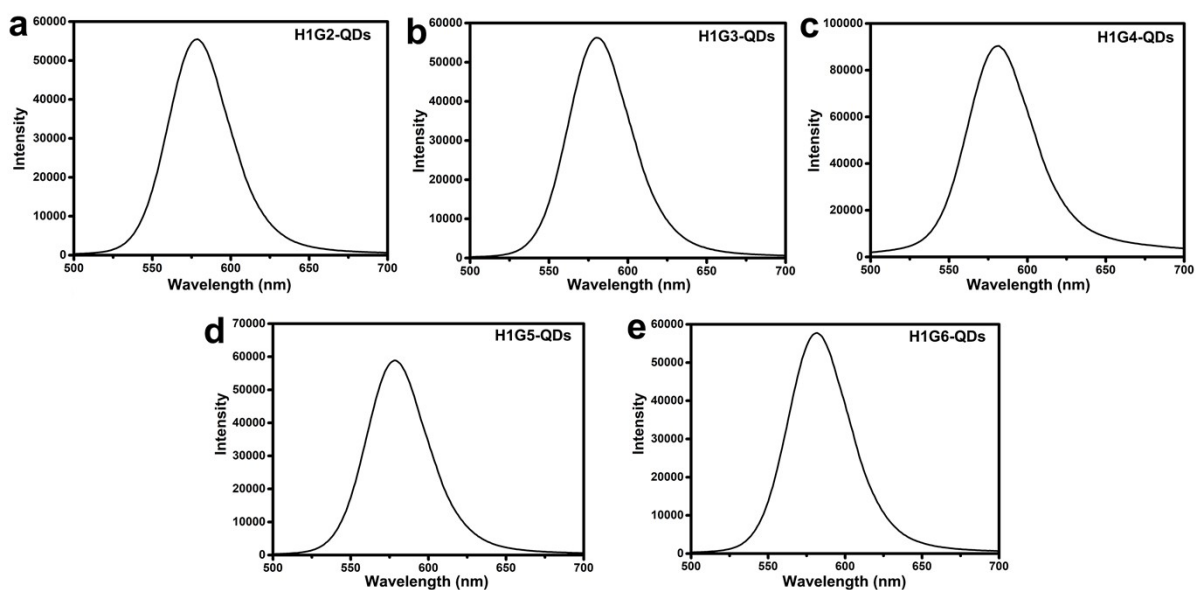
**Fig. S2.** Fluorescence spectra of H1G2-QDs (a), H1G3-QDs (b), H1G4-QDs (c), H1G5-QDs (d) and H1G6-QDs (e).

**Table S1** Physicochemical properties of HGP-QDs.

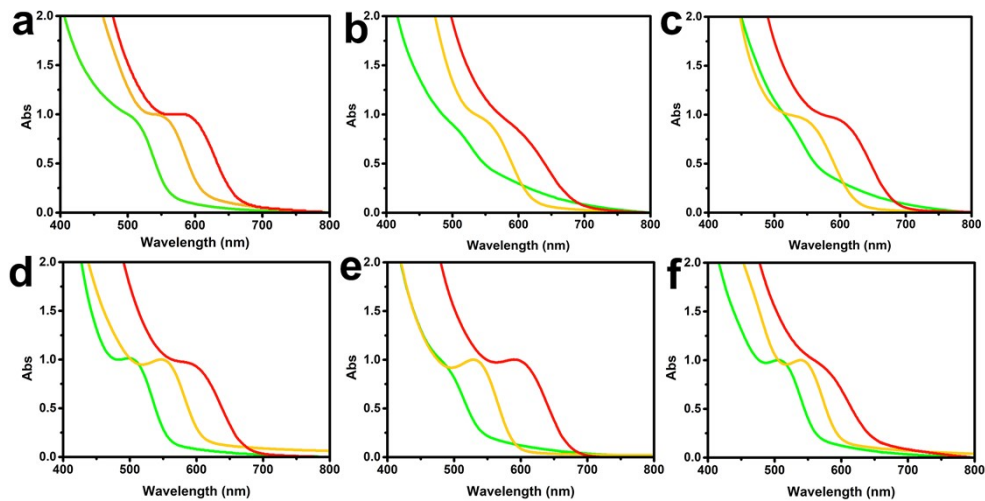| Name | $\lambda_{em}$(nm) | QY(%) | $\xi$ (mV) |
|---|---|---|---|
| | 545 | 22.0 | -30.2 |
| H1G1-QDs | 600 | 21.1 | -34.6 |
| | 655 | 6.80 | -36.9 |
| | 535 | 23.0 | -30.9 |
| H1G2-QDs | 610 | 28.1 | -33.5 |
| | 675 | 8.00 | -36.8 |
| | 550 | 21.3 | -32.8 |
| H1G3-QDs | 620 | 17.9 | -35.2 |
| | 675 | 6.25 | -38.1 |
| | 545 | 21.2 | -32.1 |
| H1G4-QDs | 600 | 19.9 | -33.5 |
| | 660 | 10.1 | -38.7 |
| | 525 | 17.4 | -29.2 |
| H1G5-QDs | 585 | 21.7 | -34.4 |
| | 640 | 13.1 | -36.5 |
| | 545 | 18.7 | -32.6 |
| H1G6-QDs | 595 | 20.1 | -34.6 |
| | 640 | 15.4 | -37.6 |

**Fig. S3.** UV-visible spectra of H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e) and H1G6-QDs (f) with three different colors (green, orange, and red).
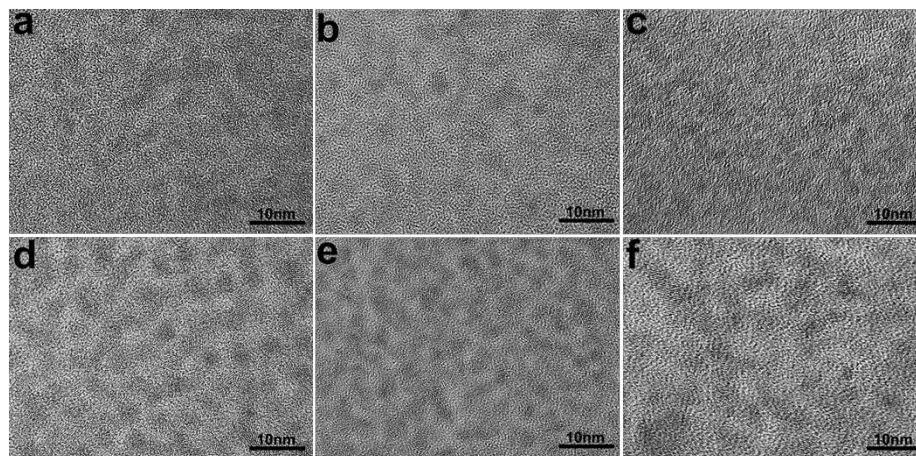


**Fig. S4.** TEM images of green HGP-QDs. H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e), and H1G6-QDs (f).
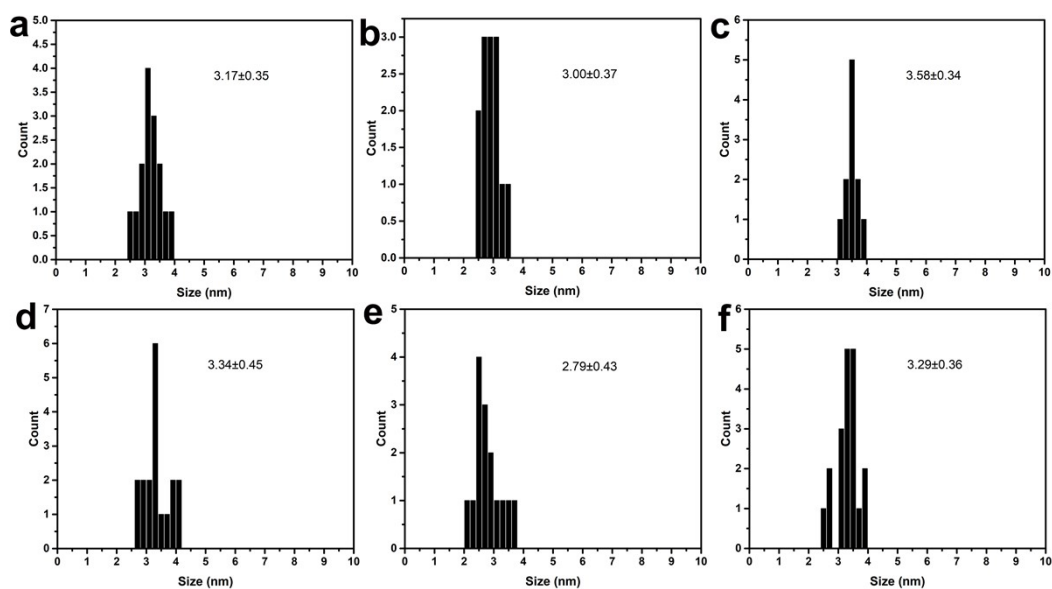


**Fig. S5.** The size distribution of green HGP-QDs. H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e), and H1G6-QDs (f).
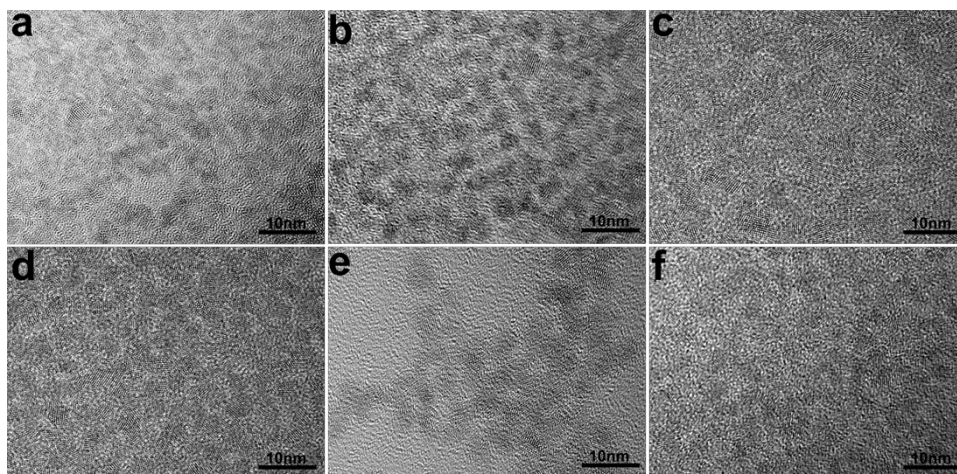
**Fig. S6.** TEM images of orange HGP-QDs. H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e), and H1G6-QDs (f).
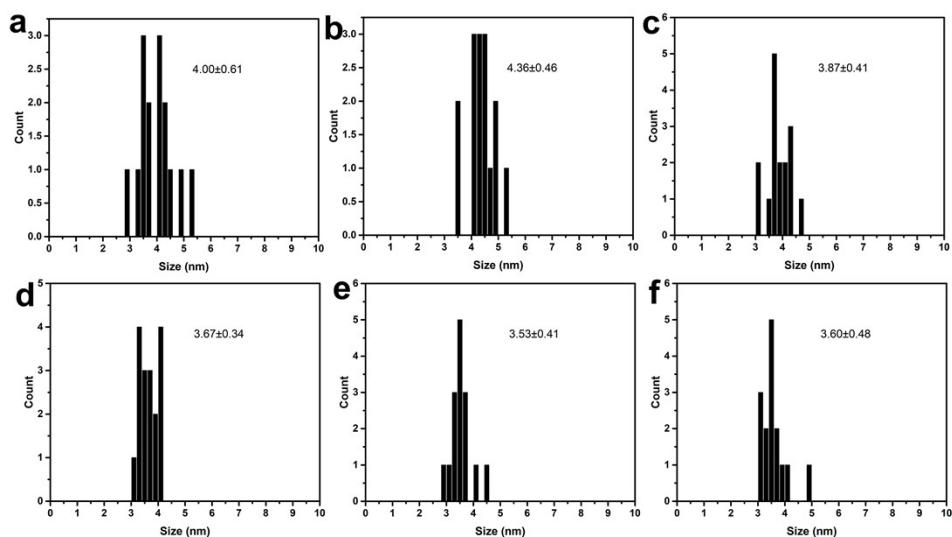


**Fig. S7.** The size distribution of orange HGP-QDs. H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e), and H1G6-QDs (f).
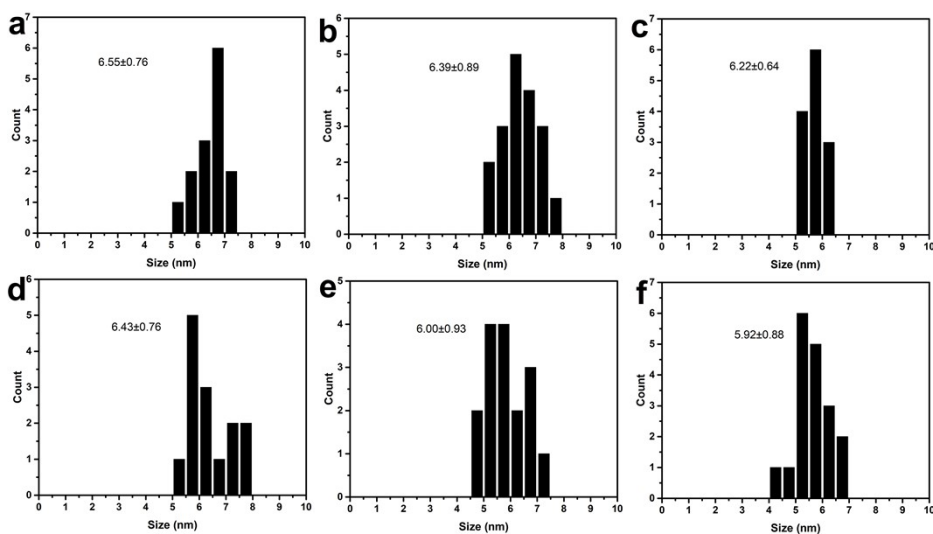


**Fig. S8.** The size distribution of red HGP-QDs. H1G1-QDs (a), H1G2-QDs (b), H1G3-QDs (c), H1G4-QDs (d), H1G5-QDs (e), and H1G6-QDs (f).
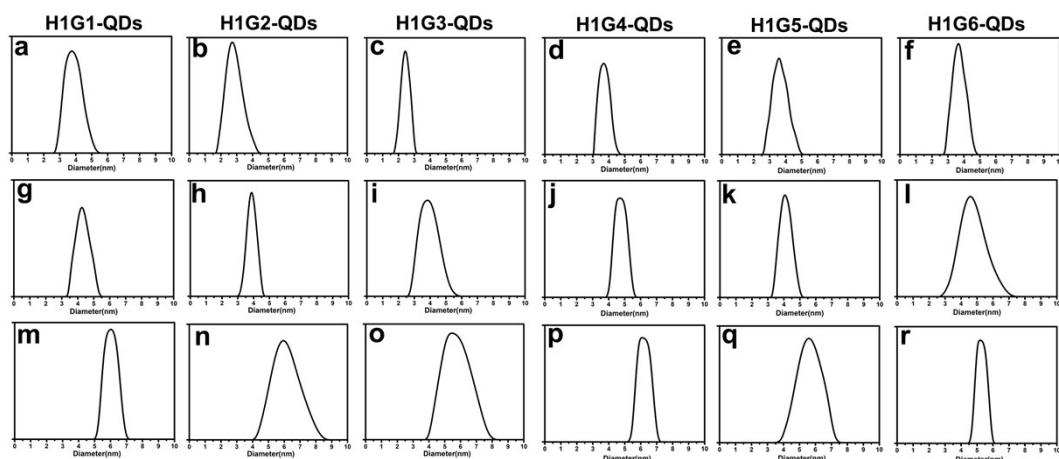
**Fig. S9.** DLS analysis of H1G1-QDs (a, g and m), H1G2-QDs (b, h and n), H1G3-QDs (c, i and o), H1G4-QDs (d, j and p), H1G5-QDs (e, k and q), and H1G6-QDs (f, l and r).
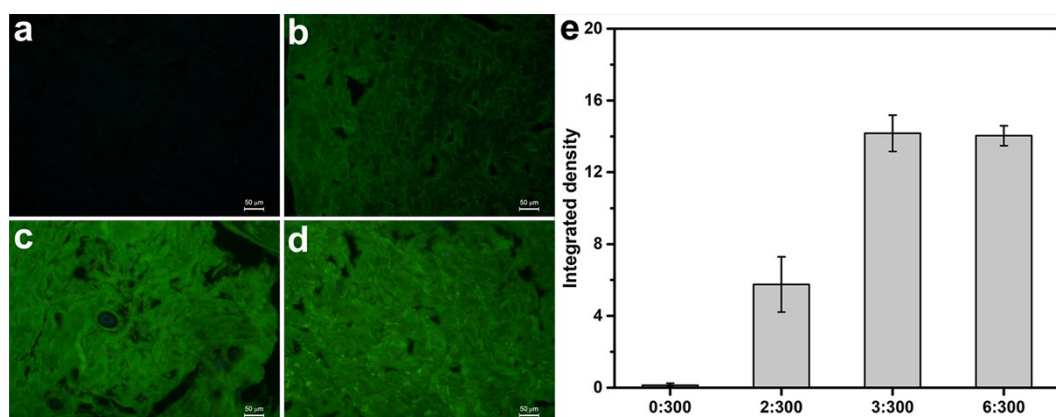


**Fig. S10.** Fluorescence micrographs of skin tissues stained with H1G1-QDs prepared with 0 (a), 0.1 (b), 0.15 (c) and 0.3 mM (d) G1, respectively. The integrated density of tissues stained with H1G1-QDs prepared with G1:H1 ratios of 0:300, 2:300, 3:300 and 6:300, representing G1 concentrations of 0, 0.1, 0.15 and 0.3 mM(e).
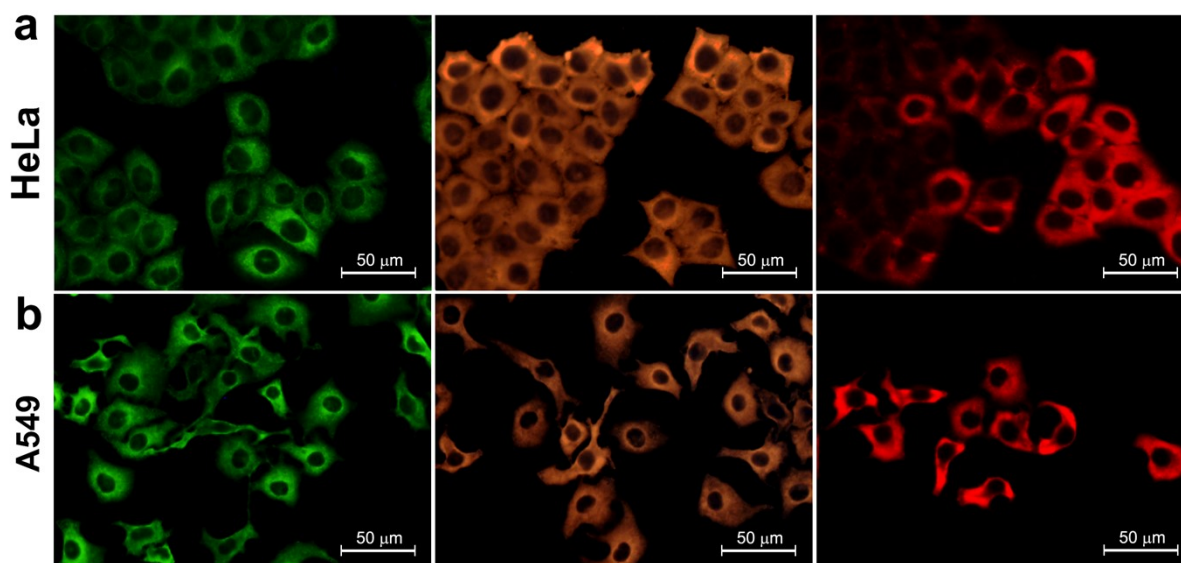


**Fig. S11.** Fluorescence micrographs of fixed HeLa cells (a) and A549 cells (b) stained with multicolor H1G4-QDs (green, orange, and red).
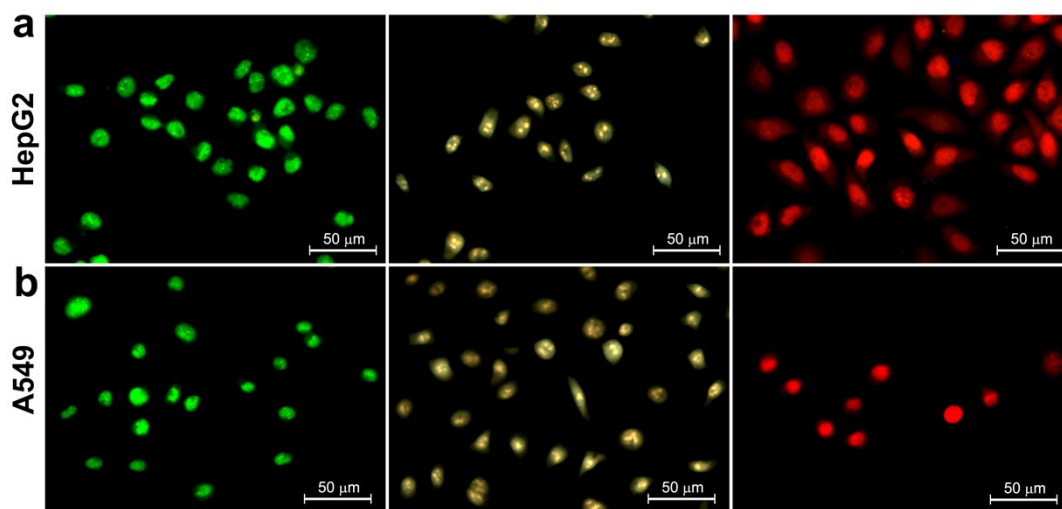
**Fig. S12.** Fluorescence micrographs of fixed HepG2 cells (a) and A549 cells (b) stained with multicolor H1G5-QDs (green, yellow, and red).
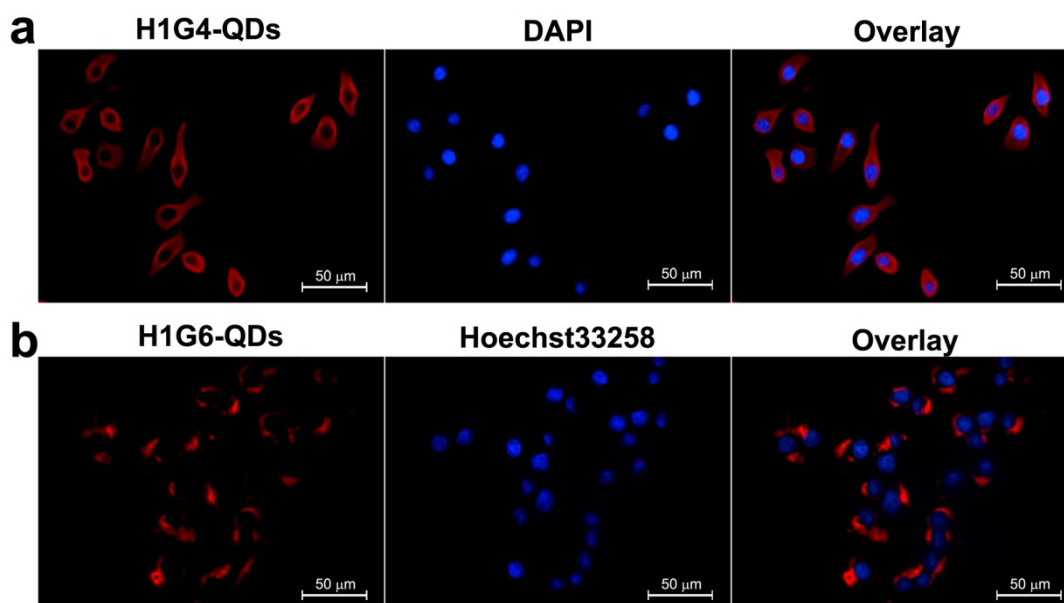


**Fig. S13.** Fluorescence micrographs of HeLa cells stained with H1G4-QDs and DAPI (a), as well as H1G6-QDs and Hoechst 33258 (b).

**Table S2.** Performance of developed methods for the construction of specific QDs probes

| Methods | One-step synthesis | Cells and tissues imaging | Multiplex imaging |
|---|---|---|---|
| Pre-synthesis QDs + Crosslink | No | Only cells | No |
| Pre-synthesis QDs + Electrostatic adsorption | No | Only cells | No |
| Pre-synthesis QDs + Assembly | No | No | No |
| MPA+Protein | Yes | Only cells | No |
| TG+His-tag-PEG | Yes | Only cells | No |
| This study | Yes | Cells and tissues | Yes |

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