Supplementary Materials

Self-doping Synthesis of Iodine-Carbon Quantum Dots for Sensitive Detection of Fe (III) and Cellular Imaging

Caption for Supplementary Materials

1.1 Materials

P-iodine-benzoic acid ($C_7H_5IO_2$), Anhydrous ethanol (C_2H_5OH), Potassium chloride (KCl), Iron (II) sulfate heptahydrate ($FeSO_4·7H_2O$), Barium chloride ($BaCl_2$), Sodium chloride (NaCl), Calcium chloride ($CaCl_2$), Iron(III) trichloride ($FeCl_3$), Copric chloride ($CuCl_2·2H_2O$), Nlckel chloride ($NiCl_2$), Zinc chloride ($ZnCl_2$), Cobalt (II) chloride ($CoCl_2$), Cadmium chloride ($CdCl_2$), Lead chloride ($PbCl_2$), Alanine, Methionine, Histidine, Serine, Tryptophan, Phenylalanine, Valine, Leucine, and Glycine. All reagents are analytical grade and used without purification. Deionized water was used to prepare all aqueous solutions. Tap water comes from local water. FBS purchased from BOVOGEN (South America), Trypsin -EDTA purchased from GIBCO, PBS purchased from Boster Biological Technology, MTT was purchased from MCE. HeLa cells were purchased from iCell Bioscience Inc.

1.2 Characterization

Transmission electron microscopy (TEM) images and the high-resolution transmission electron microscopy (HR-TEM) image were observed by FEI Tecnai G2 F20 S-TWIN. X-ray diffraction (XRD) patterns were obtained with an Empyrean using Cu K_α radiation. Fourier transform infrared (FT-IR) spectra were recorded with an Bruker Vertex-80. Ultraviolet–visible (UV-Vis) spectrum was recorded on TU-1901 at room temperature, and fluorescence (PL) spectra were recorded by RF-6000. X-ray Photoelectron Spectrometer (XPS) was performed on a Thermo Fisher Scientific K-Alpha. The fluorescence lifetime was measured with

Edinburgh Instruments, EI FLS980 Fluorescence Spectrofluorometer. Model of CO_2 constant temperature incubator is SCO6WE. The model of clean table is SW-CJ-1F. The model of the ENZYME marker tester is EPOCH2. Xenon lamp source model PLS-SXE300D, constant current 15 A. Confocal laser microscopy (LEICA SP8).

1.3 Quantum yield measurements

Utilizing quinine sulfate as standard, the ultraviolet absorption and fluorescence integral area of quinine sulfate and I-CQDs were measured at the same conditions. The quantum yield was calculated on the basis of the following equation:

$$\Phi=\Phi_R \cdot A_R \cdot F \cdot \eta^2 / A \cdot F_R \cdot \eta_R^2$$

In the formula, R refers to standard; A is the absorbance at excitation wavelength; F refers to the integral area of the fluorescence emission spectrum; η is the refractive index of solvent; Φ refers to quantum yield. The quantum yield of quinine sulfate is 0.54 at 330 nm excitation wavelength.

1.4 Cytotoxicity

The HeLa cells were seeded in a 96-well plate at a density of 1×10^4 cells per well for 24 h, followed by the incubation of I-CQDs (5, 10, 15, 20, 30, 40, 60, 80, 100, 150, and 200 μg/mL) with the cells for 24 h. The HeLa cells were cultured at 5% CO_2 and 37 ℃. Then, 20 μL of MTT (0.5 $mg \cdot mL^{-1}$) solution was added to each well. The cells were cultured for another 4 h. Removal the culture medium and MTT. Then 150 μL of DMSO was added to each well and shaken for 10 min. The absorbance of each well was measured at 570 nm. Cells without any treatment were selected as the

control group, and the survival rate of the control group was set at 100 %. The cell viability was estimated according to the equation:

$$\text{Cell viability (\%)} = OD_s/OD_u$$

Where OD_s is obtained in the presence of I-CQDs and OD_u is obtained in the absence of I-CQDs.

2.4 Synthesis of I-CQDs/PVA luminescent composite films

I-CQDs/PVA luminescent composite films were prepared by solution casting. Polyvinyl alcohol (PVA) and I-CQDs were mixed at a mass ratio of 1:10 was dissolved in 10 mL of deionized water at 70°C. Once PVA becomes fully dissolved, added 3 mL glycerin, and stir until the liquid is completely mixed. Then pour into the glass mold after ultrasonic defoaming, dry at 120□C for 10 h to prepare I-CQDs/PVA film.

		Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV): -11.8	**Peak 1:**	-11.8	100.0	5.84
Zeta Deviation (mV): 5.84	**Peak 2:**	0.00	0.0	0.00
Conductivity (mS/cm): 0.0790	**Peak 3:**	0.00	0.0	0.00
Result quality Good				

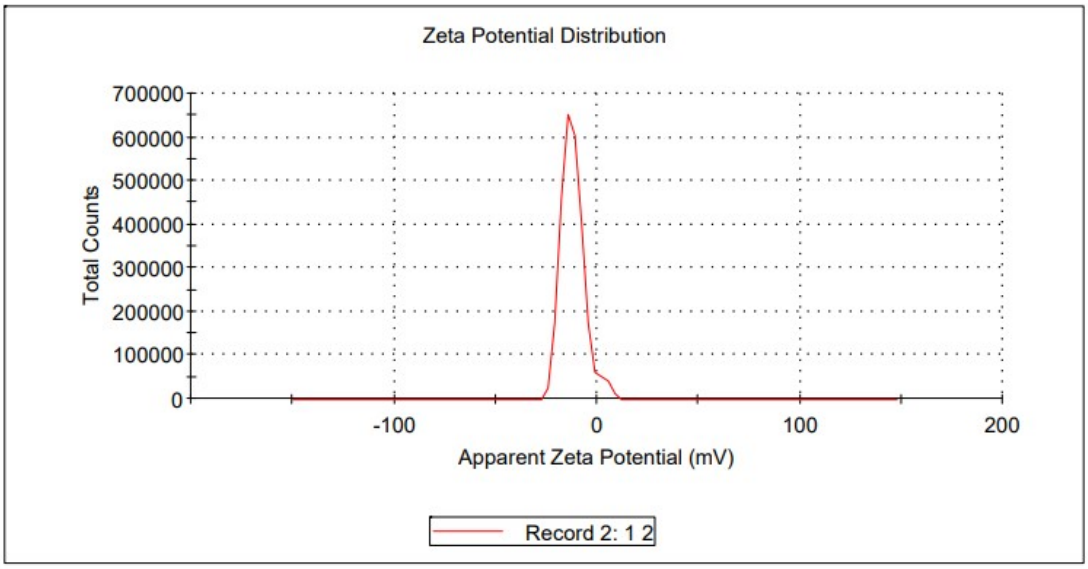

Fig. S1 Zeta potential of I-CQDs

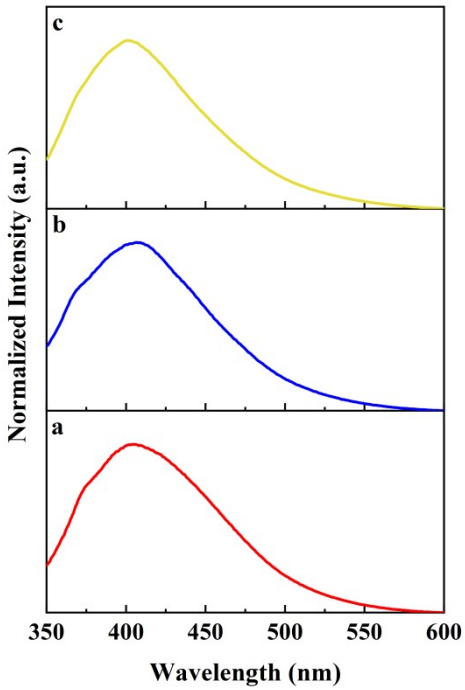

Fig. S2 The fluorescence emission spectra of I-CQDs are dispersed in water (a), ethanol (b), and ethyl acetate (c).

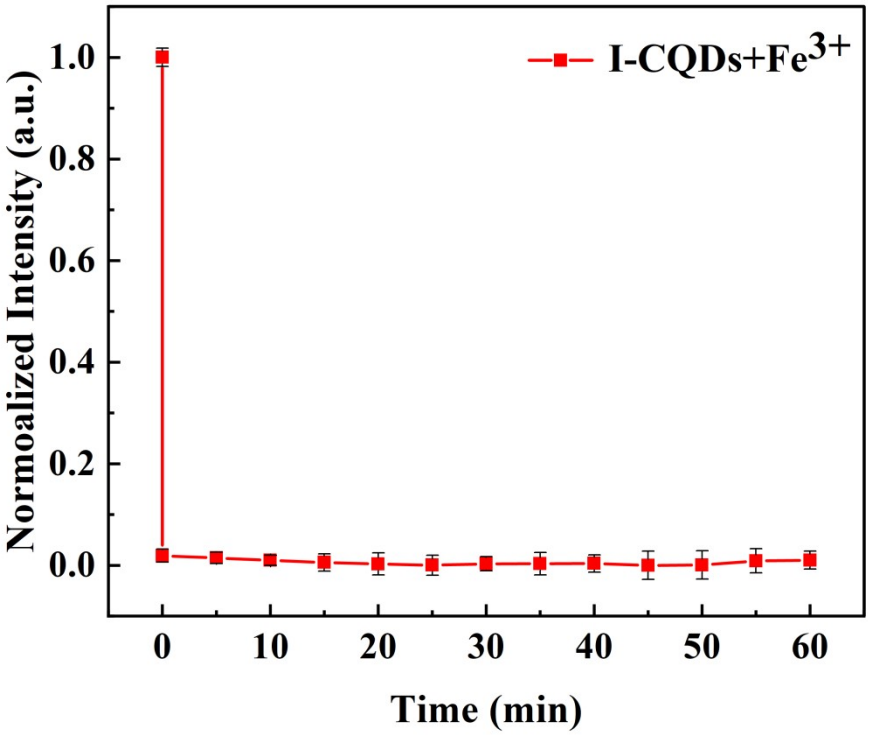

Fig.S3 Normalized intensity with annealing time.

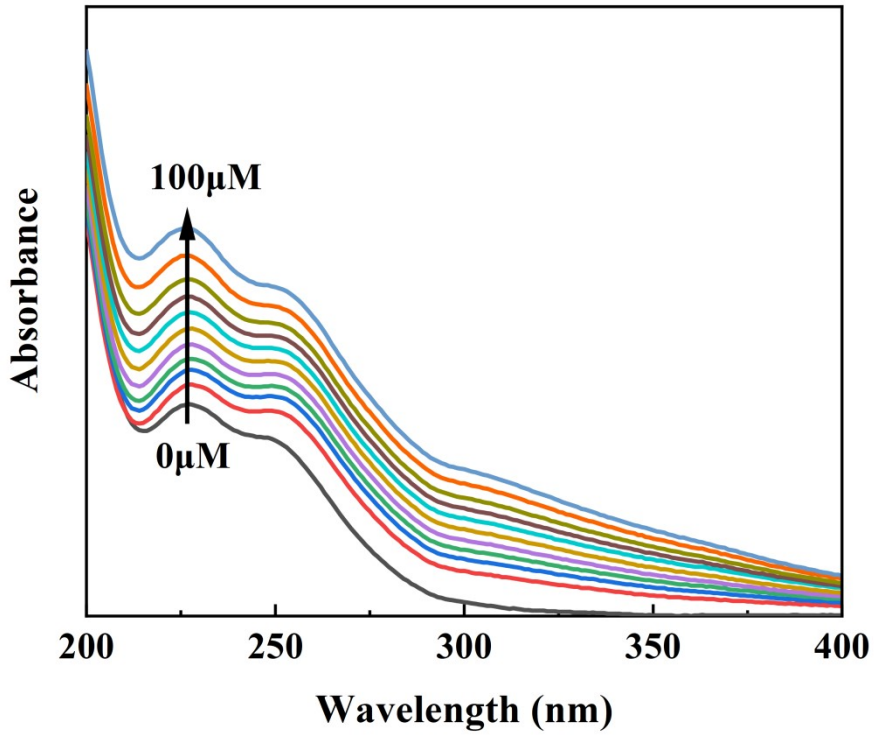

Fig. S4 UV-Vis absorption spectra of the I-CQDs with different Fe^{3+} concentration (0–100 μM).

Table S1

Comparison of fluorescence quantum yields of different iodine-doped carbon quantum dots

Surface doping	Halide source	Quantum yield	Ref.
I	Iohexol	37%	[1]
	NaI	33.8%	[2]
	KIO_3	32.4%	[3]
	Iohexol	18%	[4]
	P-iodine-benzoic acid	36.2%	This work

[1] X. Wang, Y. Lu, K. Hua, D. Yang, Y. Yang, Analytical and Bioanalytical Chemistry volume, 413 (2021) 1373-1382.
[2] Y.-S. Lin, Y. Lin, A.P. Periasamy, J. Cang, H.-T. Chang, Nanoscale Advances, 1 (2019) 2553-2561.
[3] Z. Mua, J. Huaa, Y. Yanga, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 224 (2020) 117444.
[4] H. Su, Y. Liao, F. Wu, X. Sun, H. Liu, K. Wang, X. Zhu, Colloids Surf B Biointerfaces, 170 (2018) 194-200.