Supplementary Materials

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

Caption for Supplementary Materials

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1.1 Materials

P-iodine-benzoic acid (C₇H₅IO₂), Anhydrous ethanol (C₂H₅OH), Potassium chloride (KCl), Iron (II) sulfate heptahydrate (FeSO₄·7H₂O), Barium chloride (BaCl₂), Sodium chloride (NaCl), Calcium chloride (CaCl₂), Iron(III) trichloride (FeCl₃), Copric chloride (CuCl₂·2H₂O), Nickel chloride (NiCl₂), Zinc chloride (ZnCl₂), Cobalt (II) chloride (CoCl₂), Cadmium chloride (CdCl₂), Lead chloride (PbCl₂), 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 Kα 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 CO₂ 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:

$$\Phi = \frac{\Phi_R \cdot A_R \cdot F \cdot \eta^2}{A \cdot F_R \cdot \eta_R^2}$$

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 $1 \times 10^4$ 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% CO₂ and 37 °C. Then, 20 µL of MTT (0.5 mg·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:

\[
\text{Cell viability (\%)} = \frac{OD_s}{OD_u}
\]

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.
Fig. S1 Zeta potential of I-CQDs

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zeta Potential (mV)</td>
<td>-11.8</td>
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<tr>
<td>Zeta Deviation (mV)</td>
<td>5.84</td>
</tr>
<tr>
<td>Conductivity (mS/cm)</td>
<td>0.0790</td>
</tr>
</tbody>
</table>

Peak 1: -11.8, Area (%): 100.0, St Dev (mV): 5.84
Peak 2: 0.00, Area (%): 0.0, St Dev (mV): 0.00
Peak 3: 0.00, Area (%): 0.0, St Dev (mV): 0.00

Result quality: Good
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

<table>
<thead>
<tr>
<th>Surface doping</th>
<th>Halide source</th>
<th>Quantum yield</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Iohexol</td>
<td>37%</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>NaI</td>
<td>33.8%</td>
<td>[2]</td>
</tr>
<tr>
<td></td>
<td>I</td>
<td>32.4%</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>KIO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>32.4%</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>Iohexol</td>
<td>18%</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>P-iodine-benzoic acid</td>
<td>36.2%</td>
<td>This work</td>
</tr>
</tbody>
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