One pot synthesis of high quantum yield of polyethylene glycol anchored carbon dots and functionalized with nuclear localization signal peptide for cell nucleus imaging

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Preparation of CDs@PEG

To prepare PEGylation CDs, we investigate the effect of various doses of PEG on the CDs fabrication, so the amount and ratio of citric acid (CA) and ethylenediamine (EA) besides the heating temperature and heating time were all fixed according to the literature with a little modification. 0.1, 0.3, 0.5, and 0.7 g PEG was dissolved in 20 mL deionized water separately, after that 2.5 g citric acid and 5 mL ethylenediamine were added into the solution in sequence. Then the Teflon tank was sealed in an autoclave and heated at 160 °C for 8 h. After cooling to room temperature, the solution of CDs@PEG was purified by centrifuging for 10 min at 15000 rpm and dialyzing for 24 h. CDs prepared with CA and EA only were not studied in our work as we mainly researched the PEGylation CDs. The quantum yield (QY) was employed as evaluation index in the formulation optimization, and QYs of CDs prepared with different amounts of PEG were shown in Table S1.
Table S1 QYs of different doses of PEG modified CDs in the formulation optimization.

<table>
<thead>
<tr>
<th>CA (g)</th>
<th>EA (mL)</th>
<th>PEG (g)</th>
<th>( I_c )</th>
<th>( A_c )</th>
<th>( I_s )</th>
<th>( A_s )</th>
<th>( \phi_c ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>5</td>
<td>0.1</td>
<td>609851.5</td>
<td>0.0438</td>
<td>604857.7</td>
<td>0.0446</td>
<td>55.4</td>
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<tr>
<td>2.5</td>
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<td>0.3</td>
<td>527781.0</td>
<td>0.0393</td>
<td>604857.7</td>
<td>0.0446</td>
<td>53.5</td>
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<td>2.5</td>
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<td>0.5</td>
<td>860211.3</td>
<td>0.0452</td>
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<td>0.7</td>
<td>707984.3</td>
<td>0.0458</td>
<td>604857.7</td>
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<td>61.6</td>
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</table>

\( \phi_s = 54\%, \eta_s = 1.33, \eta_c = 1.33 \), the range of emission wavelength is 380-580 nm.

Fig. S1 \(^{13}\)C NMR spectrum of CDs@PEG.

Fig. S2 Photographs of the aqueous solution of CDs@PEG under daylight (left) and
365 nm UV light illumination (right), respectively.

**Fig. S3** Effect of pH on the relative PL intensity of CDs.

**Fig. S4** The emission spectra of CDs in acids (A) and organic amines (B).

**Fig. S5** Photographs of CDs in water, acids, and organic amines under daylight.
**Fig. S6** The cytotoxicity profile of CDs@PEG after 24 h incubation with Hep G2, MCF7, A549 and L929 cells at varied concentrations.

**Fig. S7** Confocal laser scanning microscopy images of A549 cells incubated with NLS-CDs (100 μg·mL⁻¹) for 0.5, 1, and 4 h. Scale bar represents 50 μm.
Reference: