

Electronic Supplementary Information

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Open system synthesis of narrow-bandwidth red-fluorescent carbon quantum dots with a function of multi-metal ion sensing

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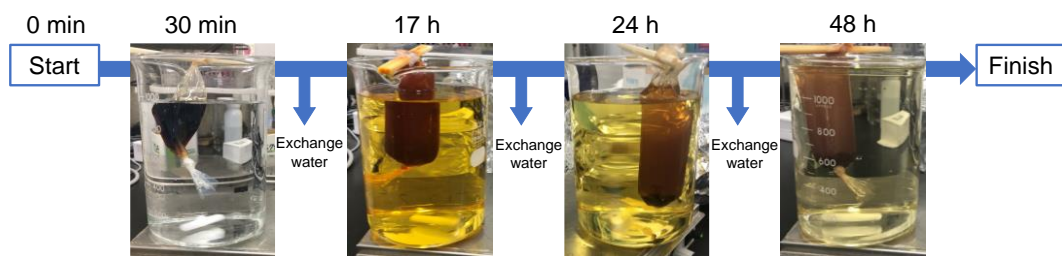
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PG-CQDs



DAR-CQDs

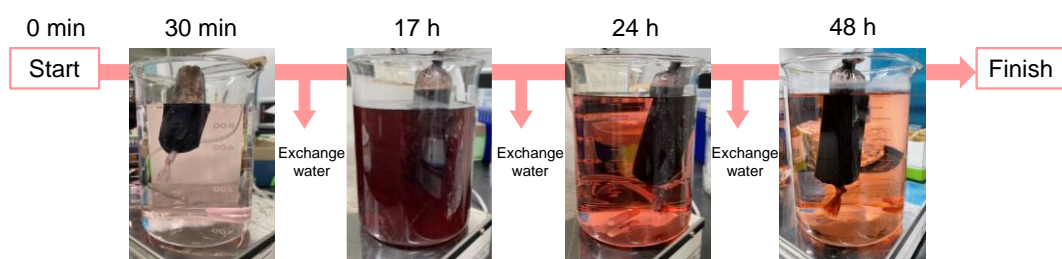


Fig. S1. Purification of PG-CQDs and DAR-CQDs by dialysis.

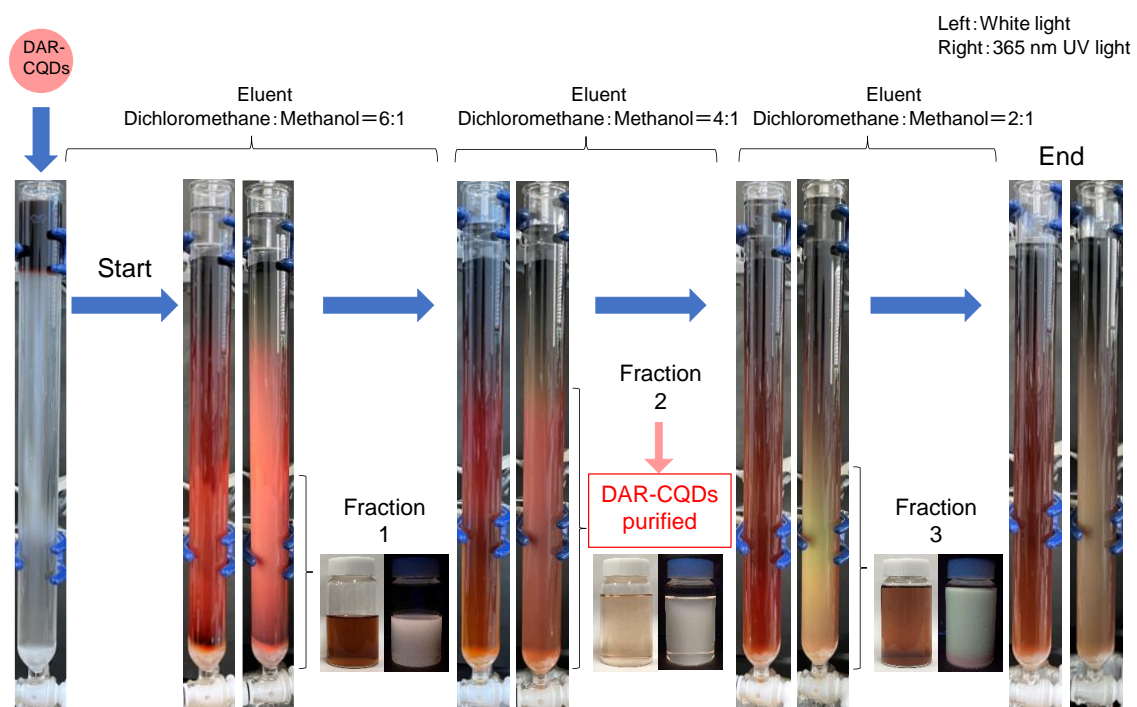
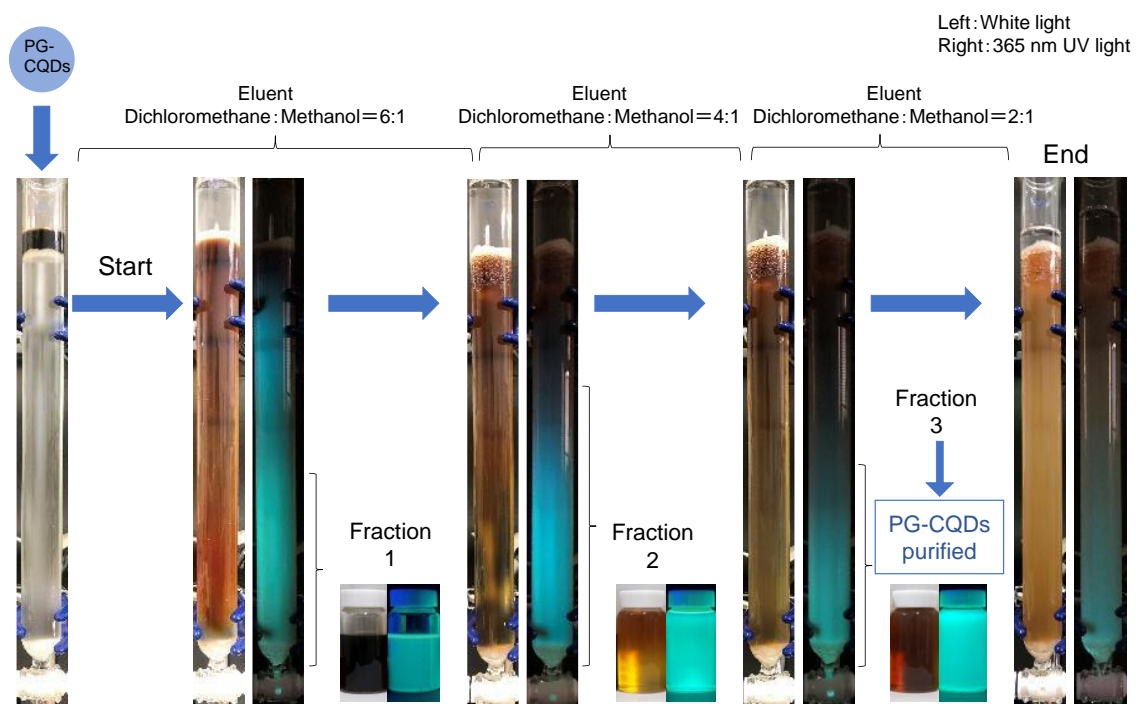


Fig. S2. Purification of PG-CQDs and DAR-CQDs by silica gel column chromatography.

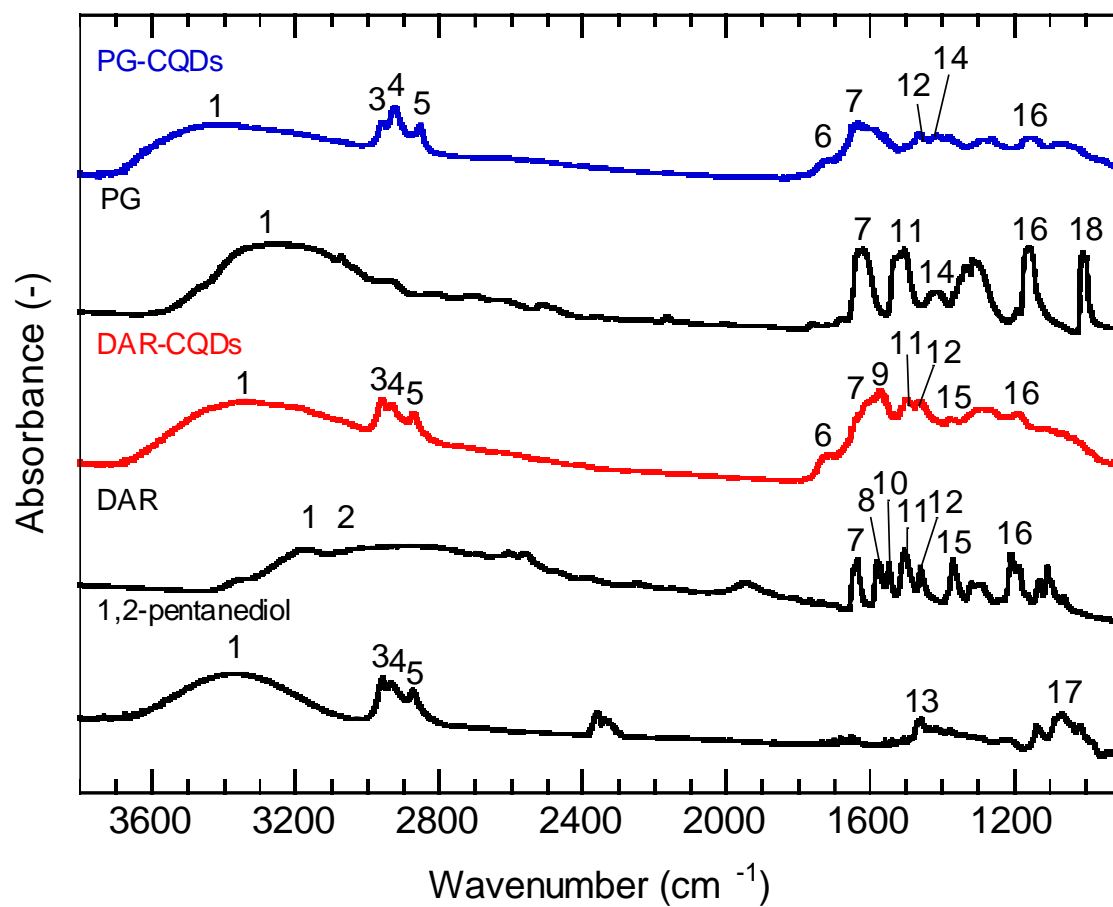


Fig. S3. FT-IR spectra of PG-CQDs, PG, DAR-CQDs, DAR, and 1,2-pentanediol.

Table S1. Assignments of FT-IR absorption peaks of Fig. S3.

Peak	Wavelength (cm ⁻¹)				Assignment	
	PG-CQDs	PG	DAR-CQDs	DAR		1,2-pentanediol
1			3100–3600		v(O–H)	
2				3100–3600	v(NH ₂)	
3	2958		2959		2959	v _{as} (CH ₃)
4	2925		2933		2934	v _s (CH ₃)
5	2872		2873		2974	v _s (CH ₂)
6	1713		1713			v(C=O)
7	1651	1622	1652	1636		ring(C=C)
8				1580		δ _{as} (NH ₃ ⁺)
9			1570			δ(NH ₂)
10				1548		δ _s (NH ₃ ⁺)
11		1506	1505	1506		ring semicircle stretching
12	1467		1468	1460		ring semicircle stretching
13					1457	δ(CH ₂)
14	1415	1418				δ(O–H)
15			1378	1370		v(C–N)
16	1160	1158	1190	1207		v(C–O)
17					1067	v _{as} (C–C–O)
18		1008				δ(C–H)

v=stretching, δ=deformation or bending, as=asymmetric, s=symmetric

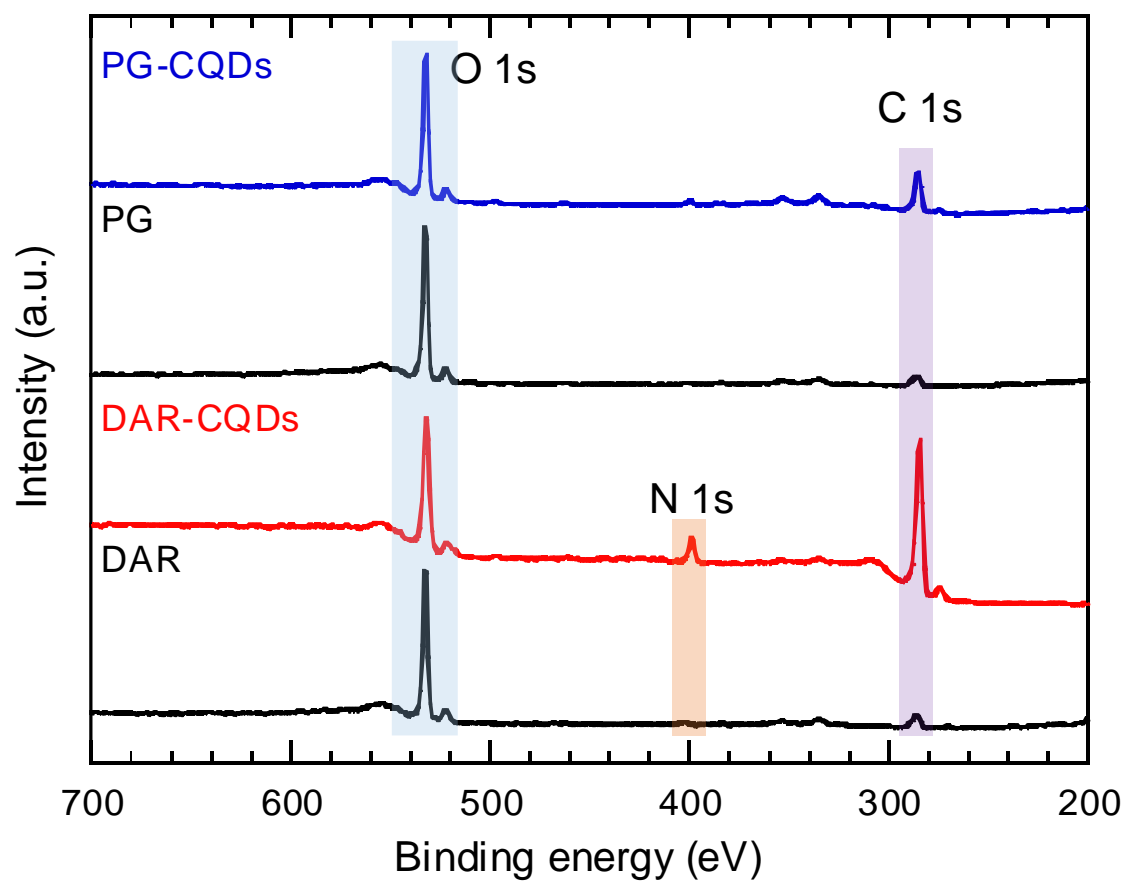


Fig. S4. XPS survey spectra of PG-CQDs, PG, DAR-CQDs, and DAR.

Table S2. Proportions of different bonds calculated from peak fitting of the C (1s) XPS spectra of PG, PG-CQDs, DAR, and DAR-CQDs.

Sample	C–OH [%]	C=C/C–C/C–N [%]
PG (Calculated)	50	50
PG (Measured)	45.9	54.1
PG-CQDs (Measured)	19.3	80.7
DAR (Calculated)	33.3	66.6
DAR (Measured)	27.3	72.7
DAR-CQDs (Measured)	1.5	89.5

Calculated: obtained from molecular structure.

Measured: obtained from peak fitting of C (1s) XPS spectrum.

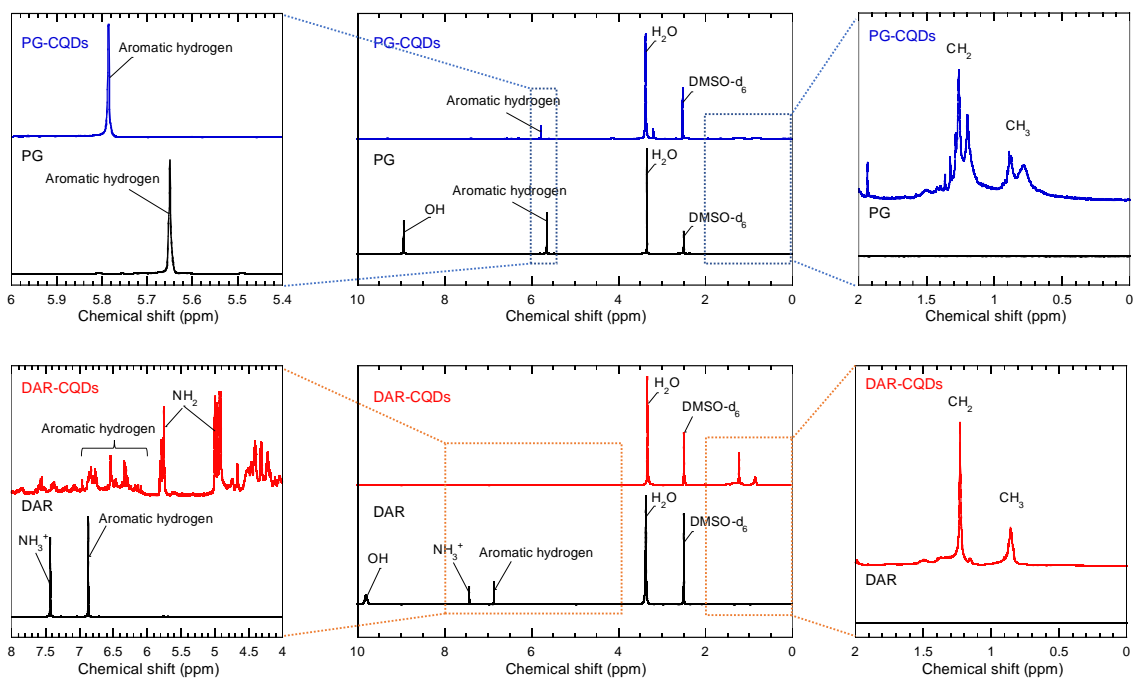


Fig. S5. $^1\text{H-NMR}$ spectra of PG-CQDs and DAR-CQDs.

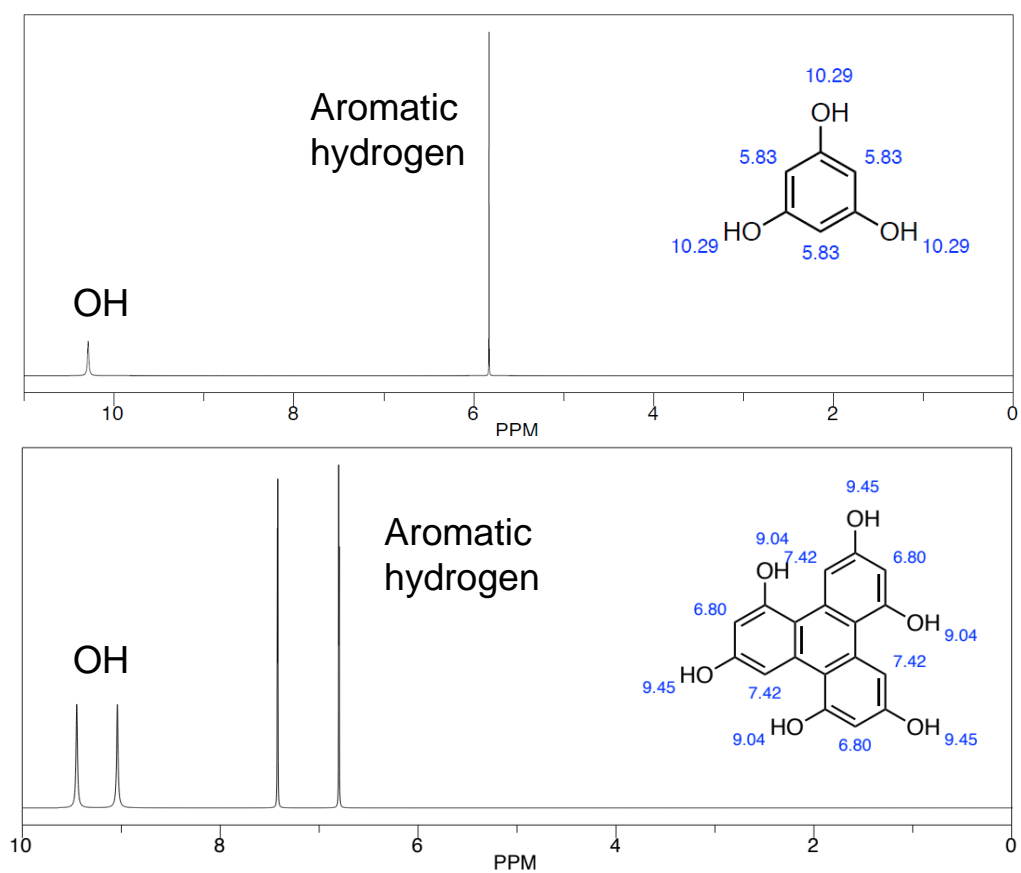


Fig. S6. Simulated $^1\text{H-NMR}$ spectra of PG and the molecule formed by dehydration

condensation of three PG molecules.

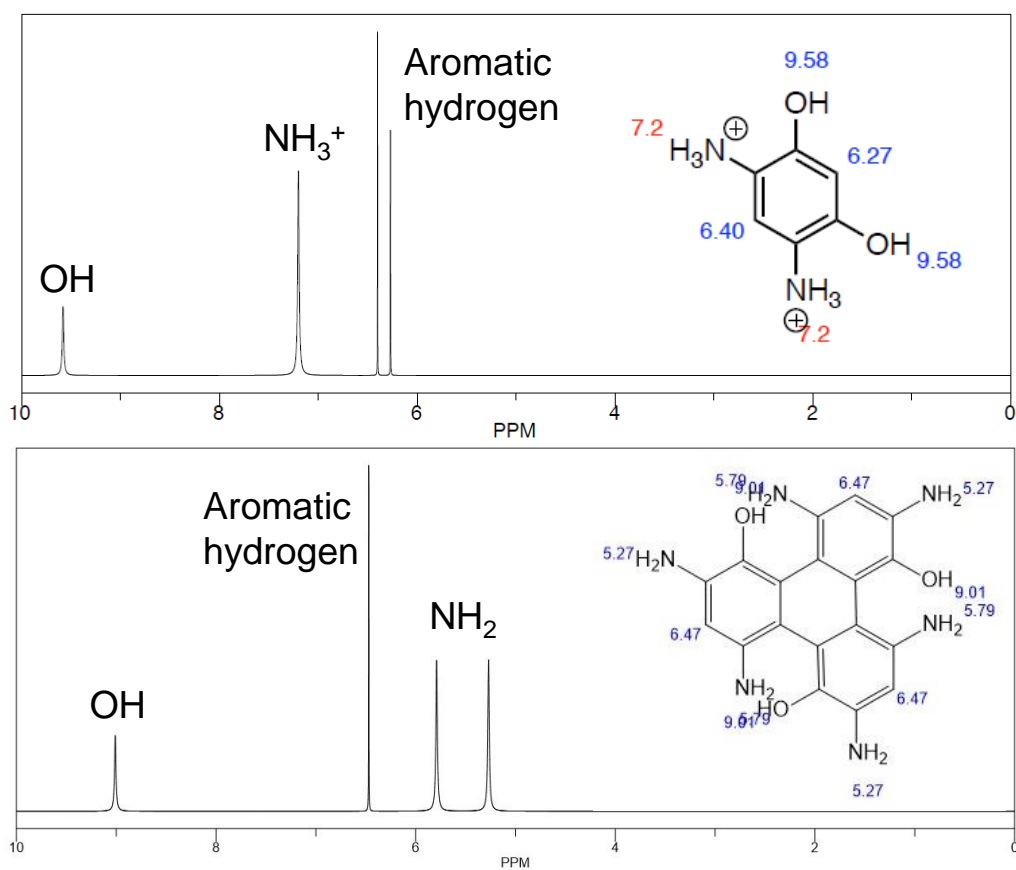


Fig. S7. Simulated $^1\text{H-NMR}$ spectra of DAR and the molecule formed by dehydration

condensation of three DAR molecules.

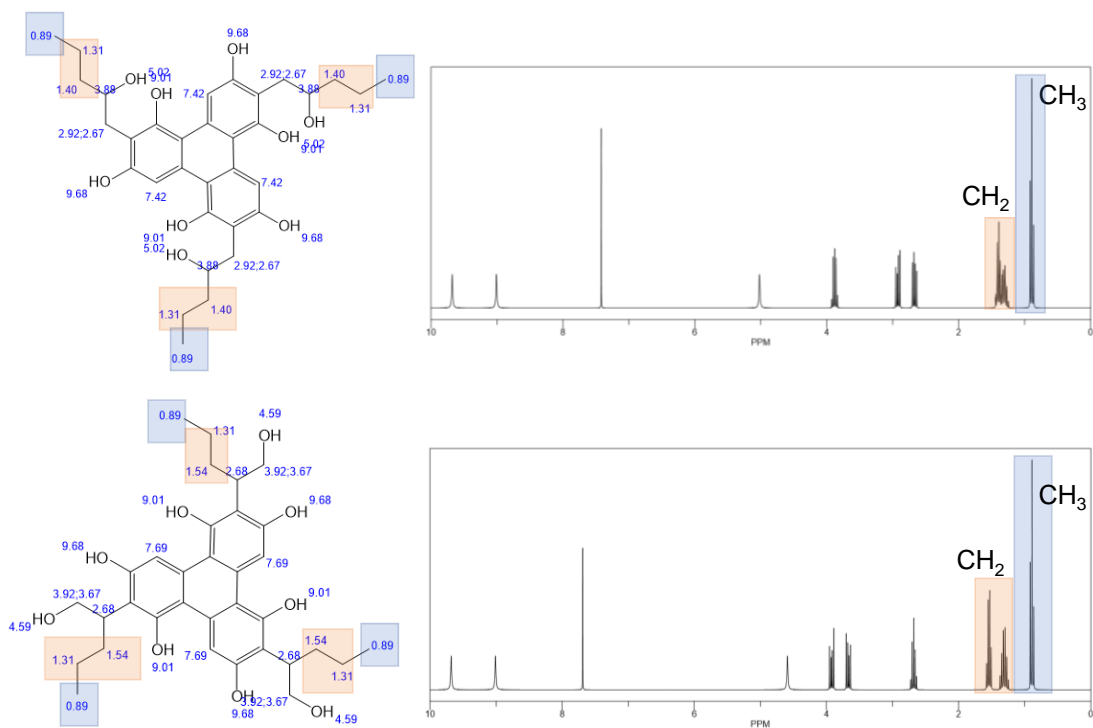


Fig. S8. Simulated $^1\text{H-NMR}$ spectra of the dehydration-condensed structure of three PG molecules bonded to three 1,2-pentanediol molecules.

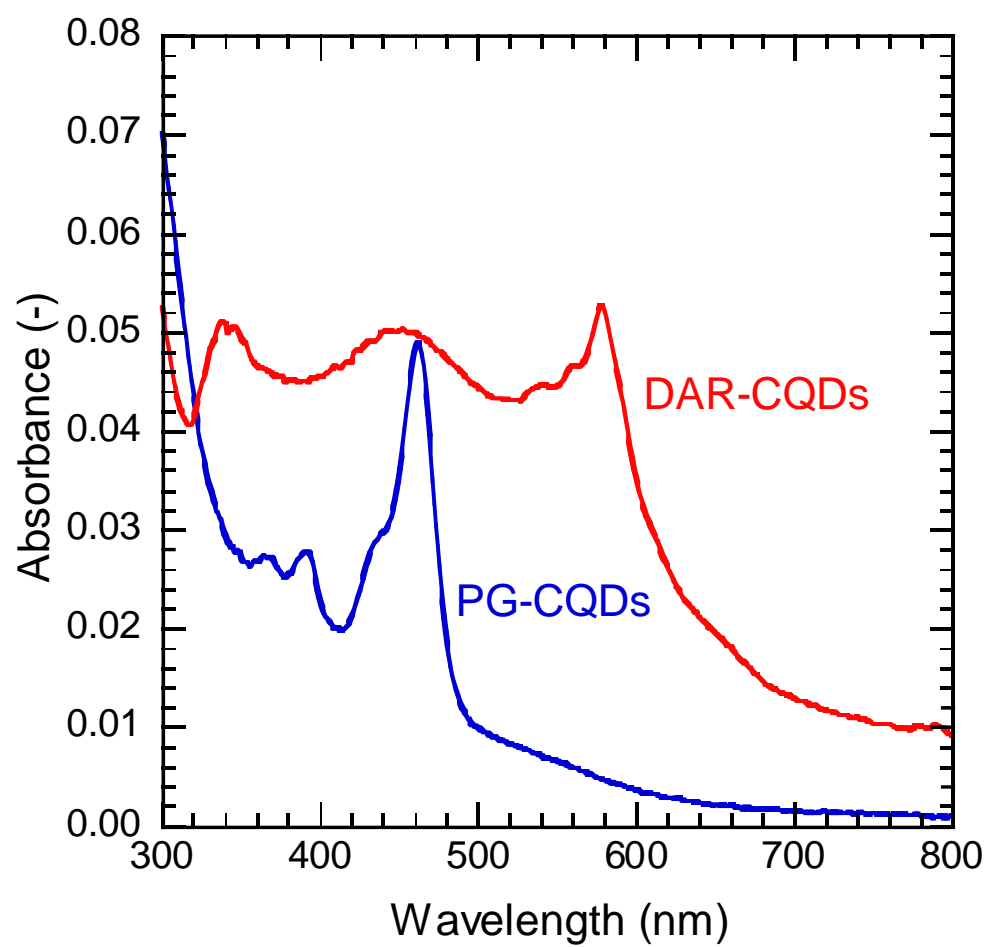


Fig. S9. UV-vis spectra of ethanol dispersions of PG-CQDs and DAR-CQDs.

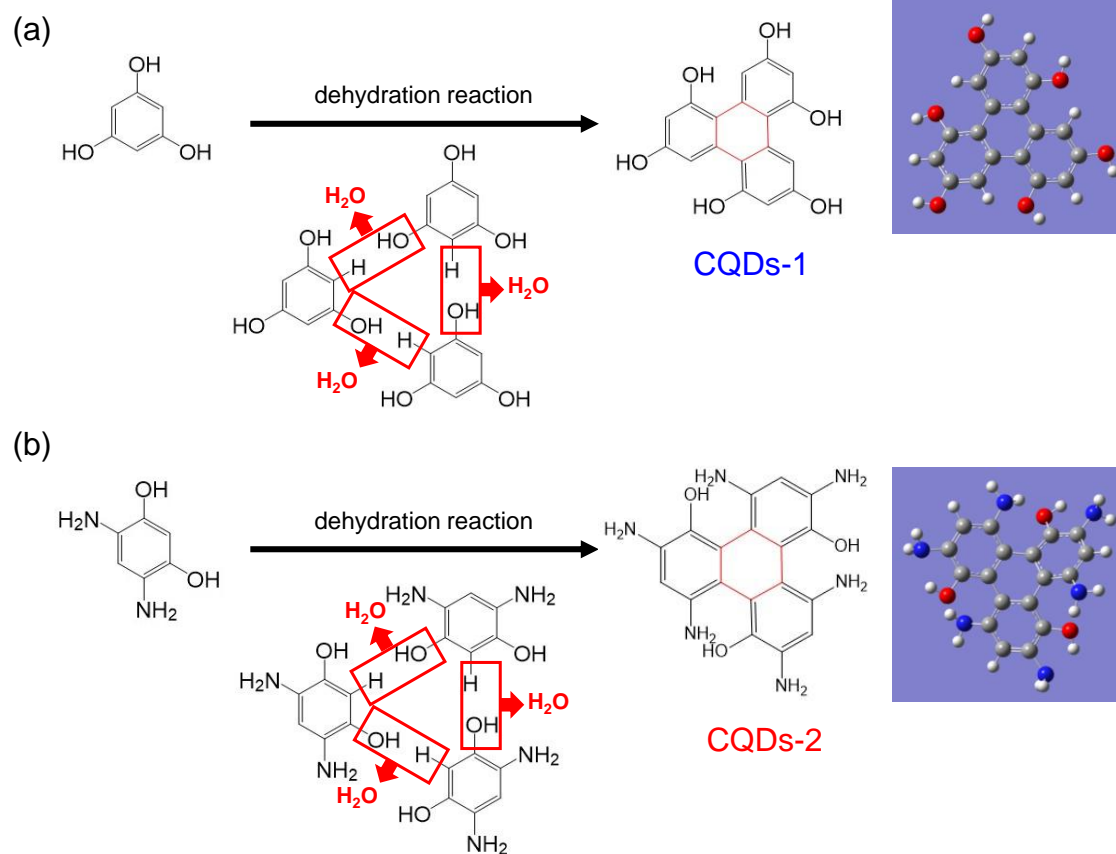


Fig. S10. Structural models and optimized structures of CQDs-1 and CQDs-2.

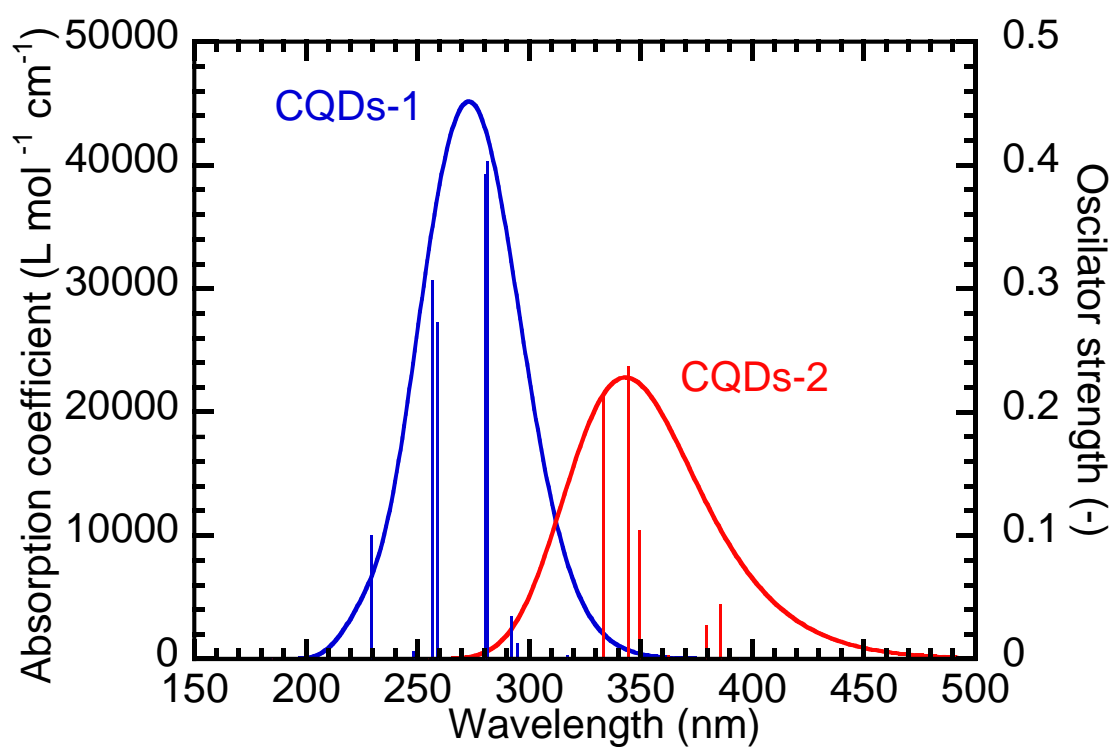


Fig. S11. UV-vis absorption spectra with oscillator strength (vertical lines) of CQDs-1 and CQDs-2 obtained by TD-DFT calculations.

Table S3. HOMO/LUMO energy levels and HOMO-LUMO energy gaps E_{H-L} of CQDs-1, CQDs-2, and CQDs-3.

Sample	HOMO (eV)	LUMO (eV)	E_{H-L} (eV)	E_{H-L} (nm)
CQDs-1	-5.044	-0.487	4.557	272
CQDs-2	-4.349	-0.543	3.806	326
CQDs-3	-4.352	-0.890	3.462	358

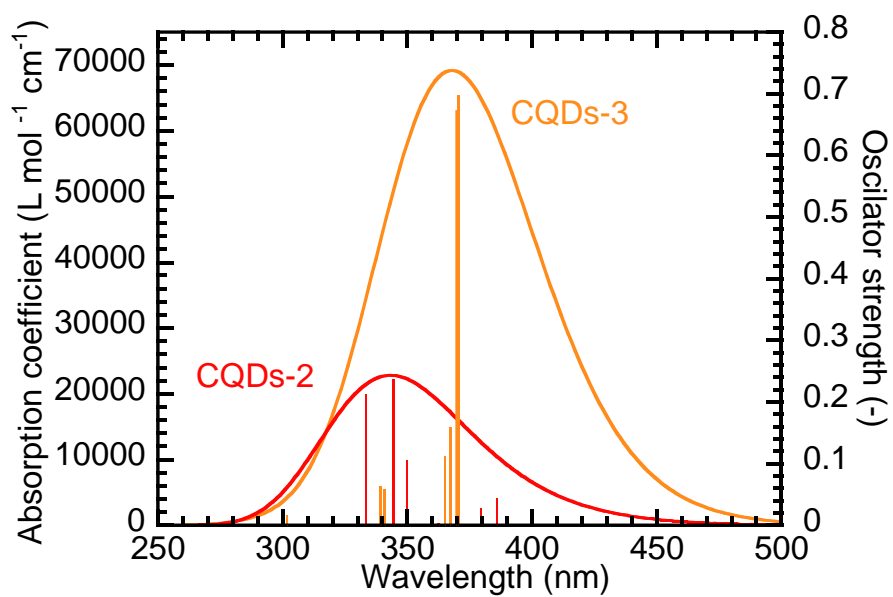
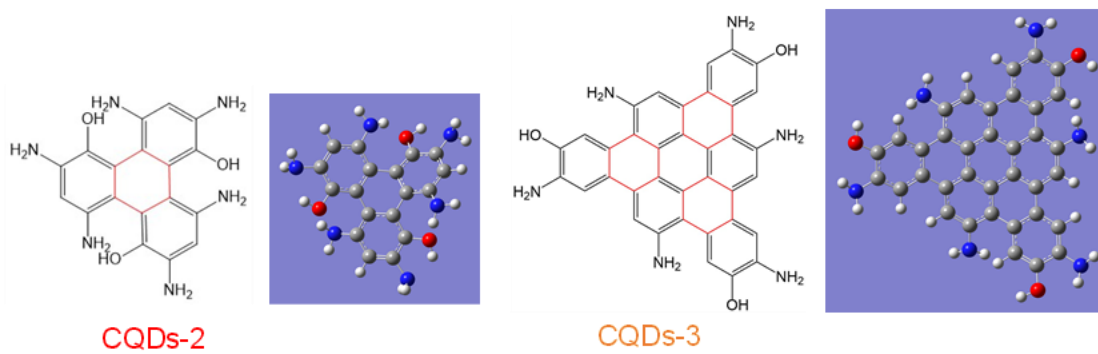


Fig. S12. Structural models and optimized structures of CQDs-2 and CQDs-3, and their UV-vis absorption spectra with oscillator strength (vertical lines) obtained by TD-DFT calculations.

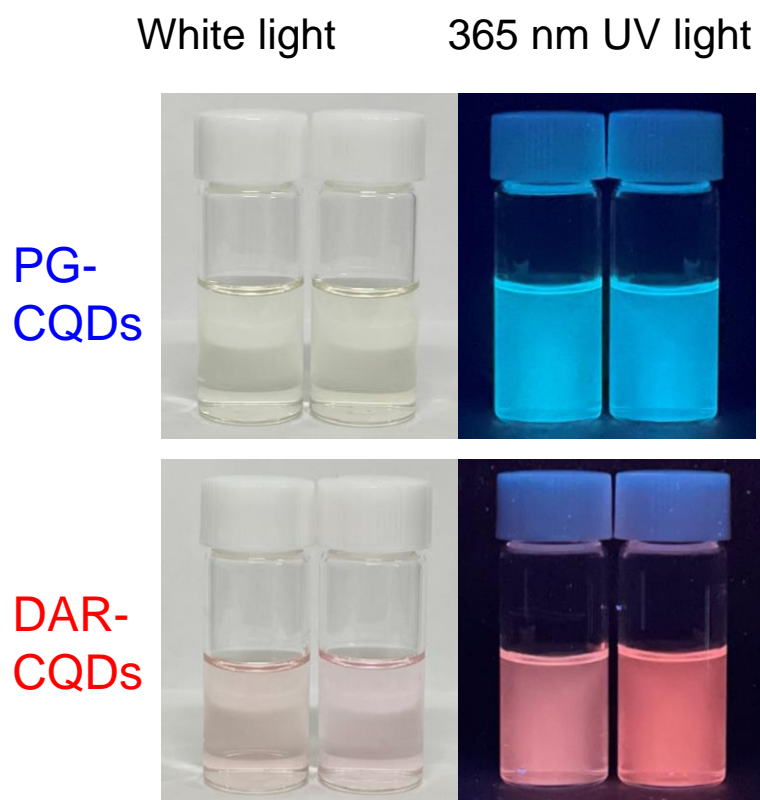


Fig. S13. Photographs of PG-CQDs and DAR-CQDs dispersions in methanol (left) and deuterated methanol (right).

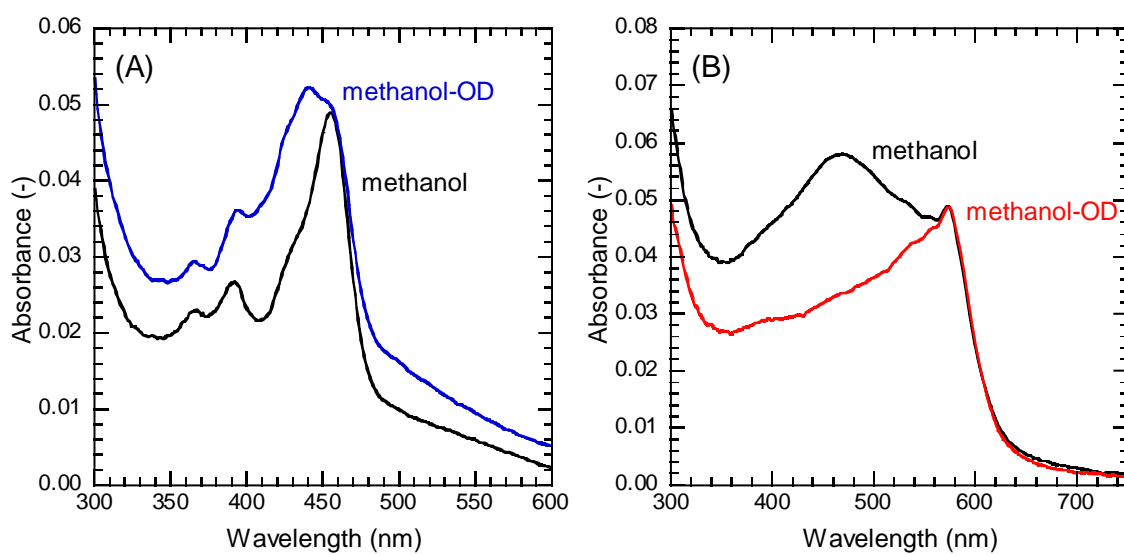


Fig. S14. UV-vis spectra of (A) PG-CQDs and (B) DAR-CQDs dispersions in methanol and deuterated methanol.

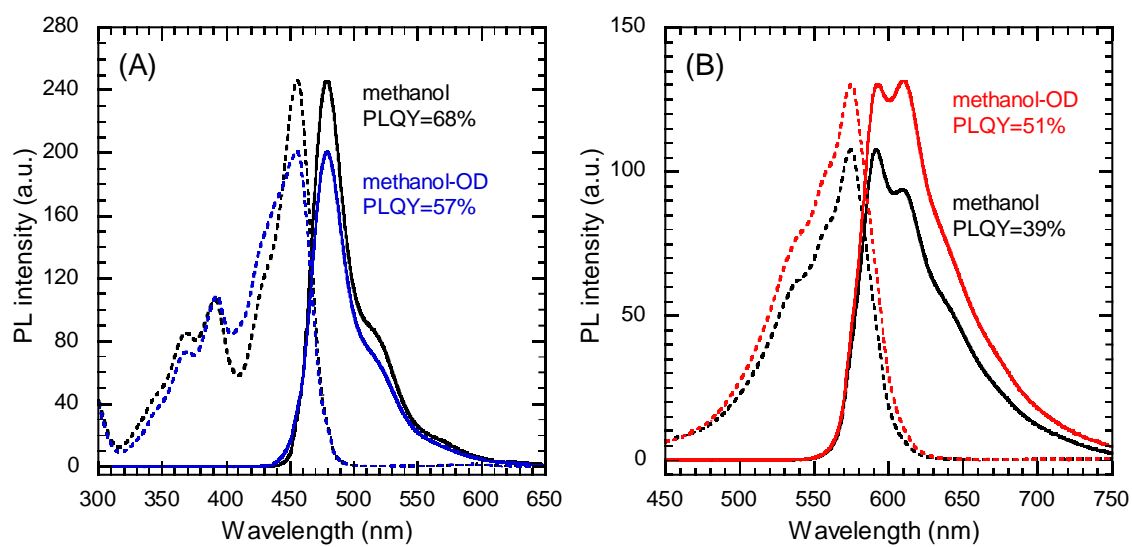


Fig. S15. PLE and PL spectra of (A) PG-CQDs and (B) DAR-CQDs dispersions in methanol and deuterated methanol.

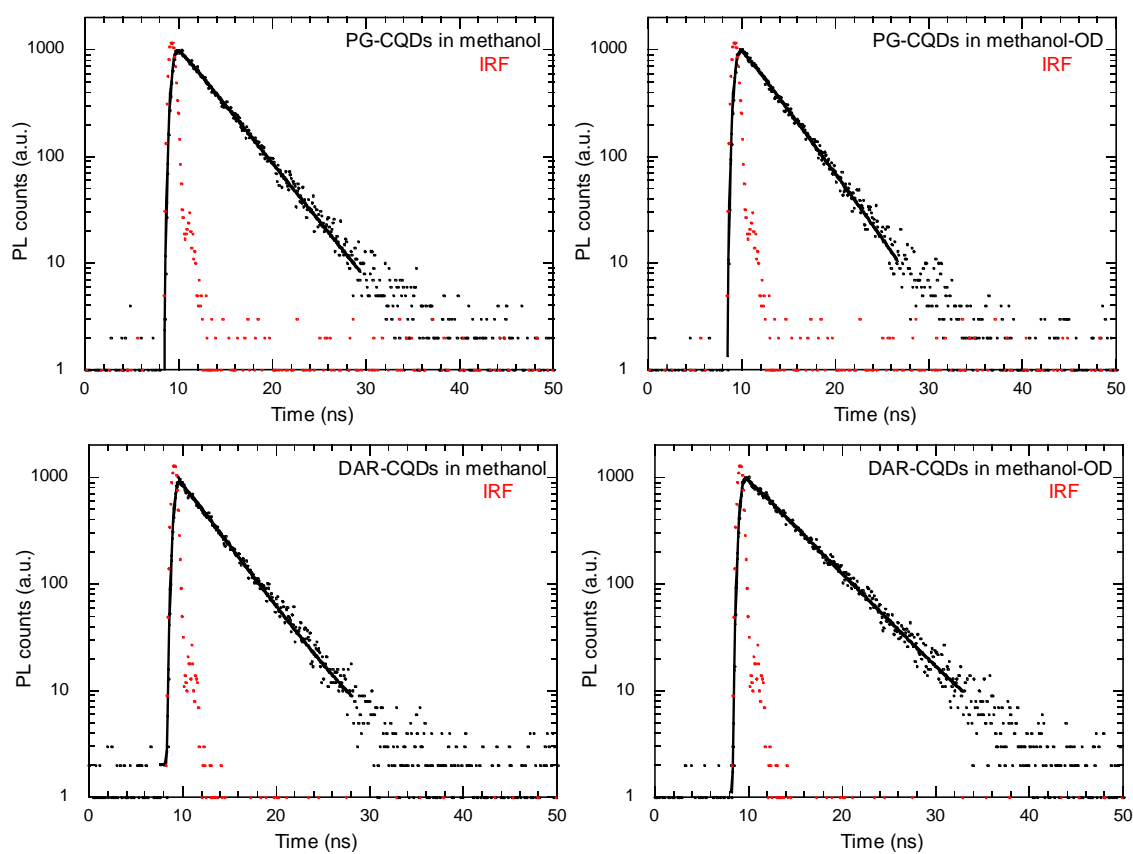


Fig. S16. PL decay curves of PG-CQDs and DAR-CQDs dispersions in methanol and deuterated methanol. λ_{ex} : PG-CQDs 405 nm, DAR-CQDs 590 nm.

Table S4. PLQYs of PG-CQD and DAR-CQD ethanol dispersions before and after storage for 26 months in the dark at room temperature.

Sample	Storage duration (month)	PLQY
PG-CQDs	0	56
	26	53
DAR-CQDs	0	30
	26	32

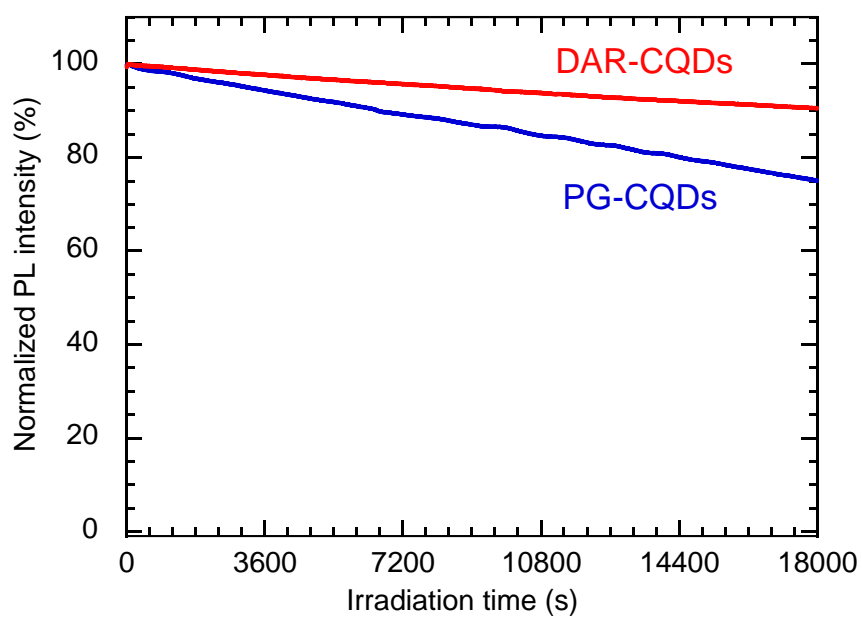


Fig. S17. Changes in PL intensities of PG-CQD and DAR-CQD ethanol dispersions with the irradiation time measured under each optimum excitation wavelength.

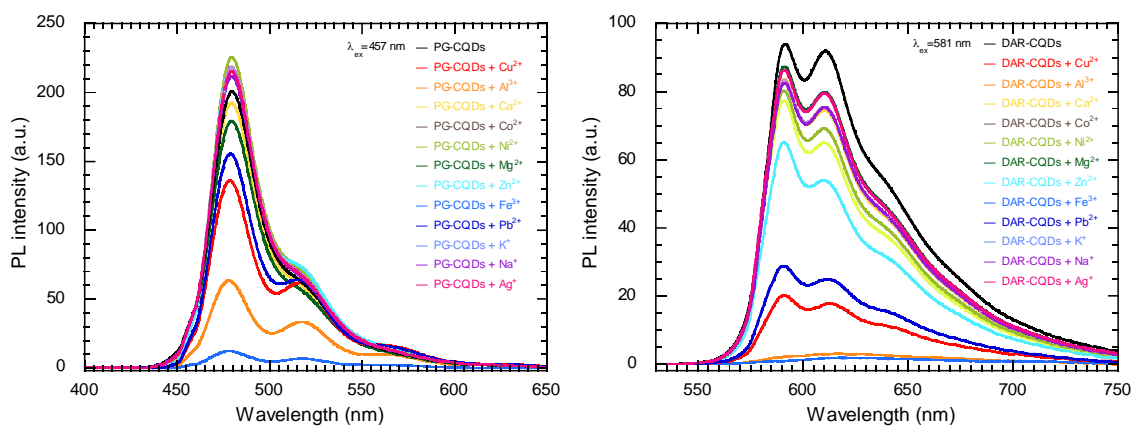


Fig. S18. The PL spectra of PG-CQDs and DAR-CQDs aqueous dispersions in the

absence and presence of different metal ions.