

Comprehensive exploration of long-wave emission carbon dots for brain tumor visualization

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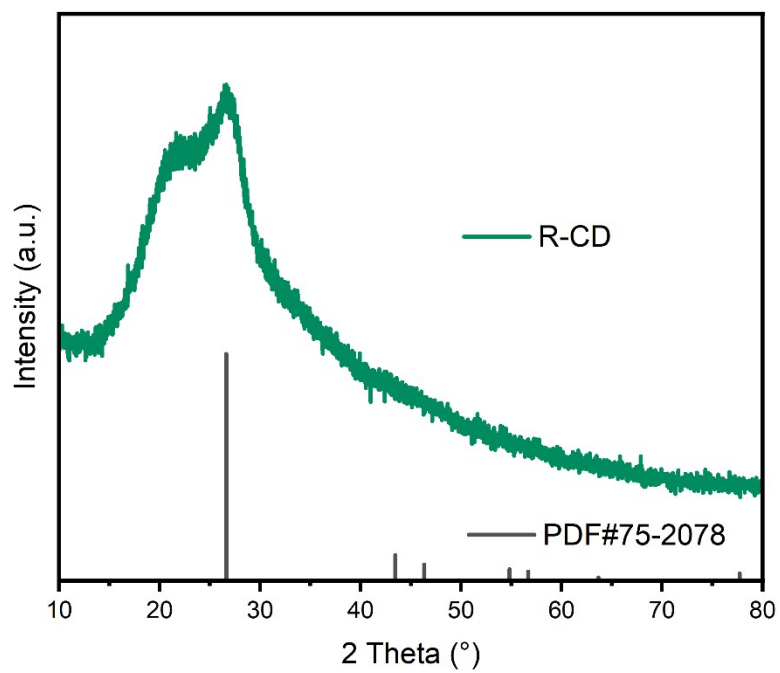


Figure S1 XRD pattern of R-CD

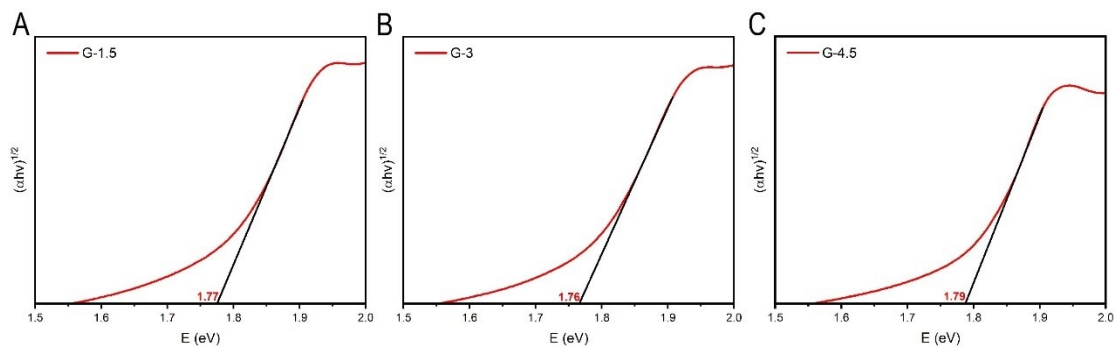


Figure S2 Bandgap of G-1.5, G-3, and G-4.5

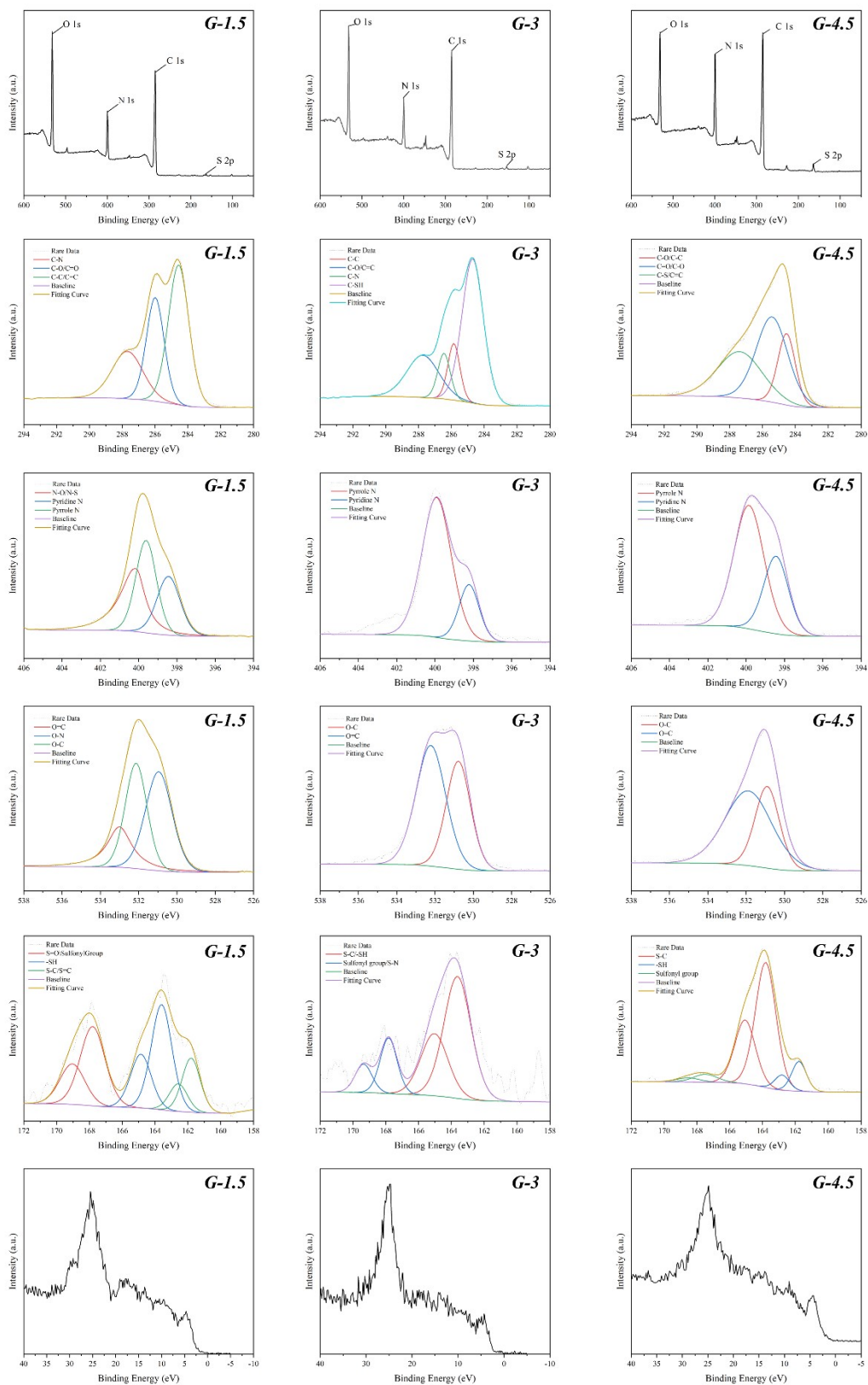


Figure S3 XPS spectra of G-1.5, G-3, and G-4.5 (Top: Survey spectrum, C 1s, N 1s, O 1s, S 2p, VB)

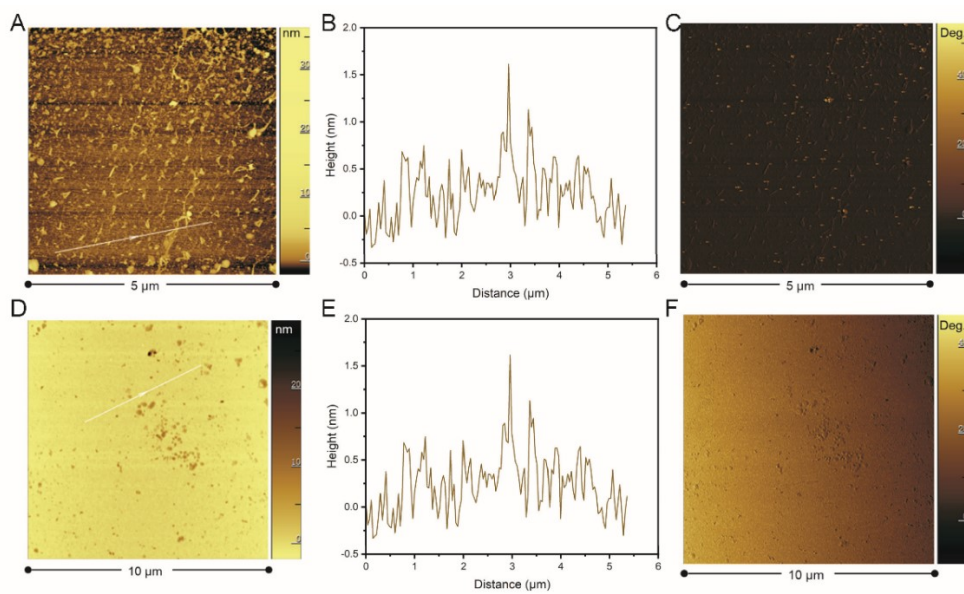


Figure S4 Typical AFM tapping mode images of R-CD with scanning probes of 7 nm (A, B, C) and 2 nm (D, E, F)

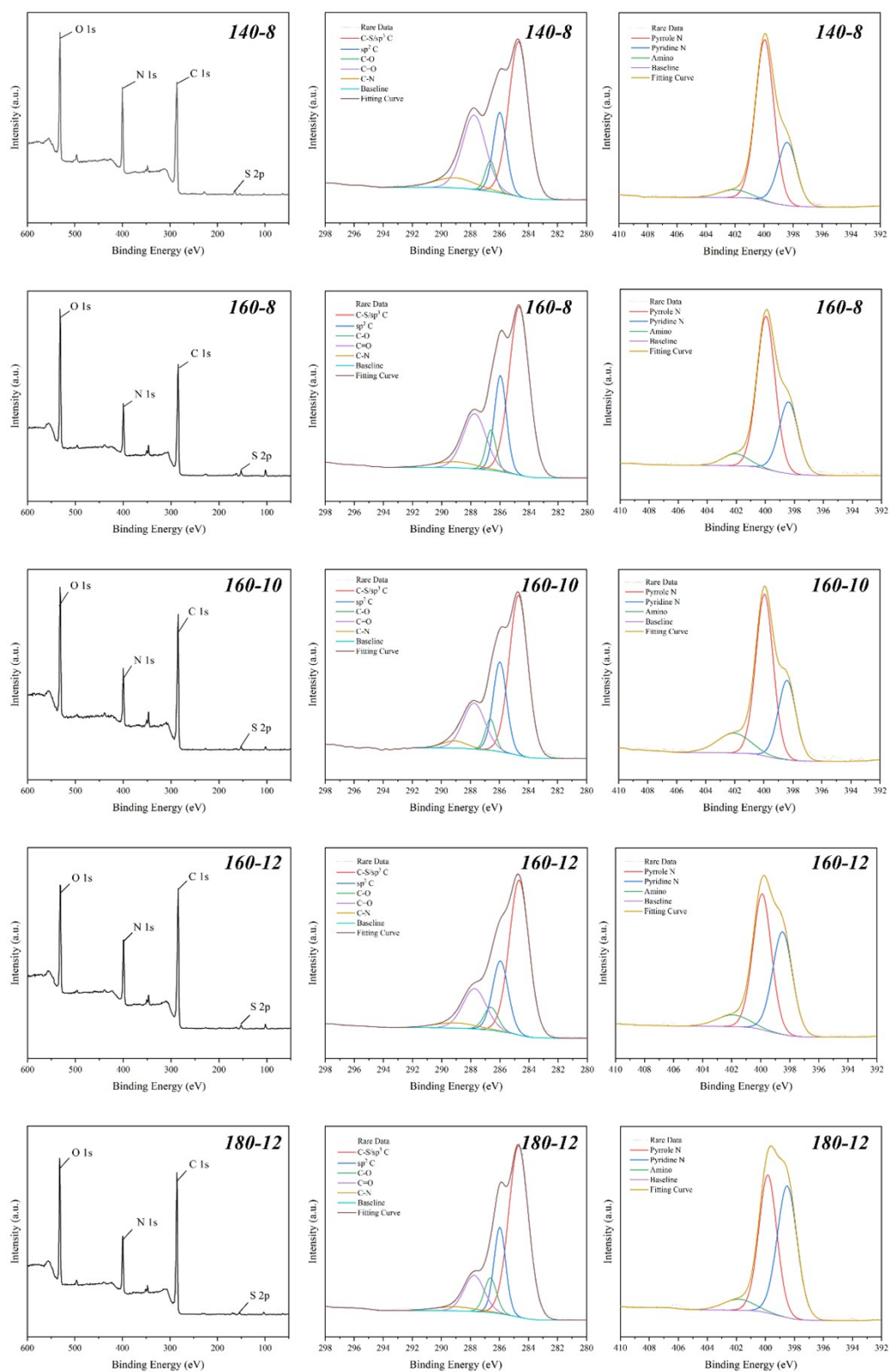


Figure S5 (A) XPS spectra of R-CD under different synthetic conditions (Left: Survey spectrum, C 1s, N 1s)

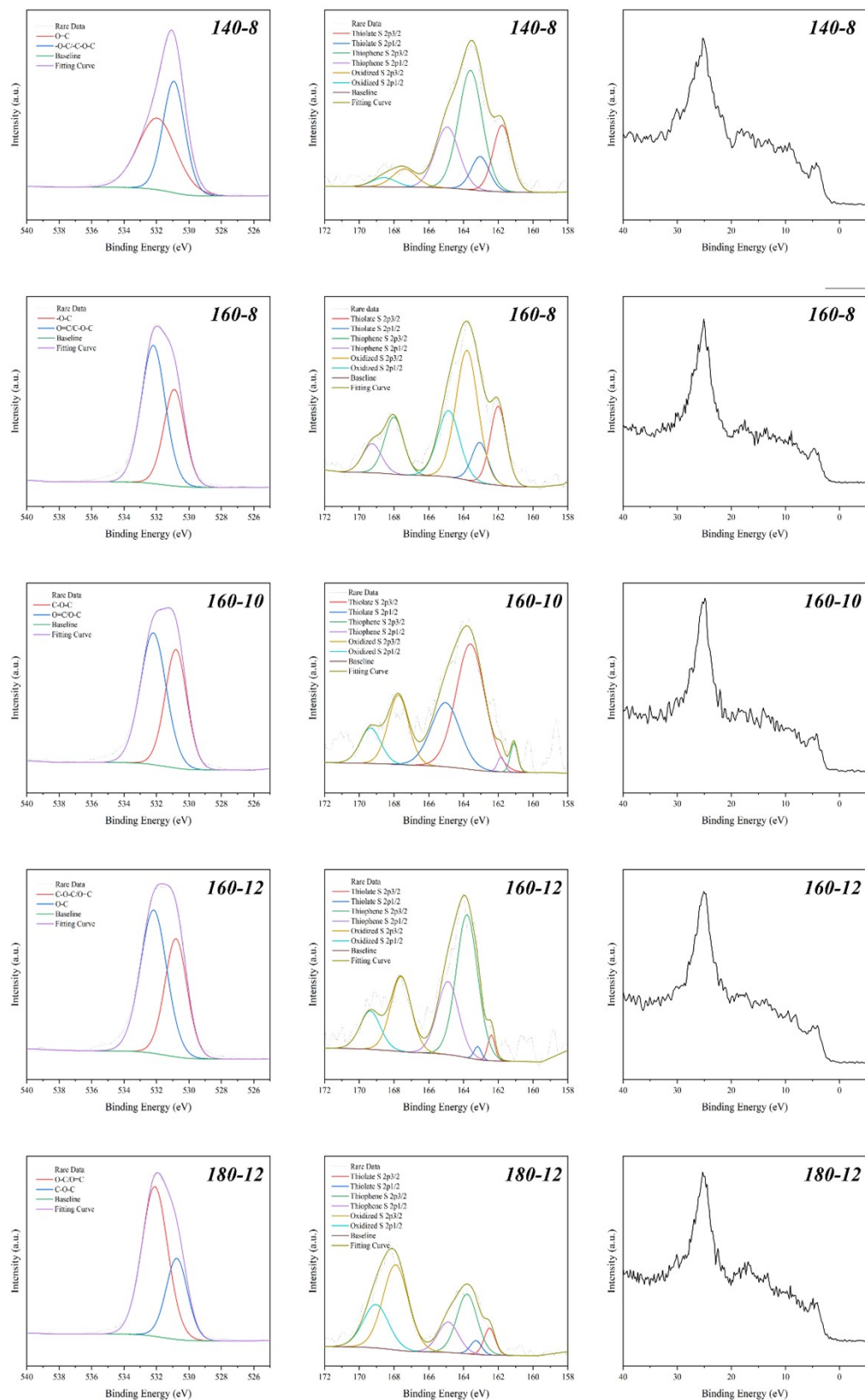


Figure S5 (B) XPS spectra of R-CD under different synthetic conditions (Left: O 1s, S 2p, VB)

Table S1 Element composition ratio and XPS valence band

| | C | N | O | S | VB/HOMO |
|---------------|----------|----------|----------|----------|----------------|
| 140-8 | 62.12% | 18.21% | 18.45% | 1.23% | 2.28 eV |
| 160-8 | 62.14% | 13.53% | 23.40% | 0.93% | 2.55 eV |
| 160-10 | 66.89% | 11.84% | 20.71% | 0.56% | 2.59 eV |
| 160-12 | 63.93% | 16.87% | 18.74% | 0.47% | 2.45 eV |
| 180-12 | 63.59% | 15.28% | 20.45% | 0.67% | 2.66 eV |

Table S2 XPS analysis of C 1s

| | sp³ C | sp² C | C-O | C=O | C-N |
|---------------|-------------------------|-------------------------|------------|------------|------------|
| 140-8 | 46.51% | 15.81% | 4.65% | 26.51% | 6.51% |
| 160-8 | 52.36% | 18.32% | 6.28% | 19.37% | 3.66% |
| 160-10 | 52.08% | 21.35% | 5.73% | 17.71% | 3.13% |
| 160-12 | 54.05% | 19.46% | 5.95% | 16.76% | 3.78% |
| 180-12 | 59.17% | 17.75% | 7.69% | 12.43% | 2.96% |

Table S3 XPS analysis of N 1s

| | Pyrrole N | Pyridine N | Amino |
|---------------|------------------|-------------------|--------------|
| 140-8 | 67.30% | 26.96% | 5.74% |
| 160-8 | 62.03% | 30.54% | 7.43% |
| 160-10 | 64.38% | 28.02% | 7.60% |
| 160-12 | 55.17% | 39.44% | 5.38% |
| 180-12 | 40.44% | 55.41% | 4.15% |

Table S4 XPS analysis of S 2p

| | Thiolate S | Thiophene S | Oxidized S |
|---------------|-------------------|--------------------|-------------------|
| 140-8 | 27.20% | 63.18% | 9.62% |
| 160-8 | 24.64% | 20.65% | 54.71% |
| 160-10 | 68.64% | 4.55% | 26.82% |
| 160-12 | 3.81% | 63.98% | 32.20% |
| 180-12 | 8.08% | 33.85% | 58.08% |

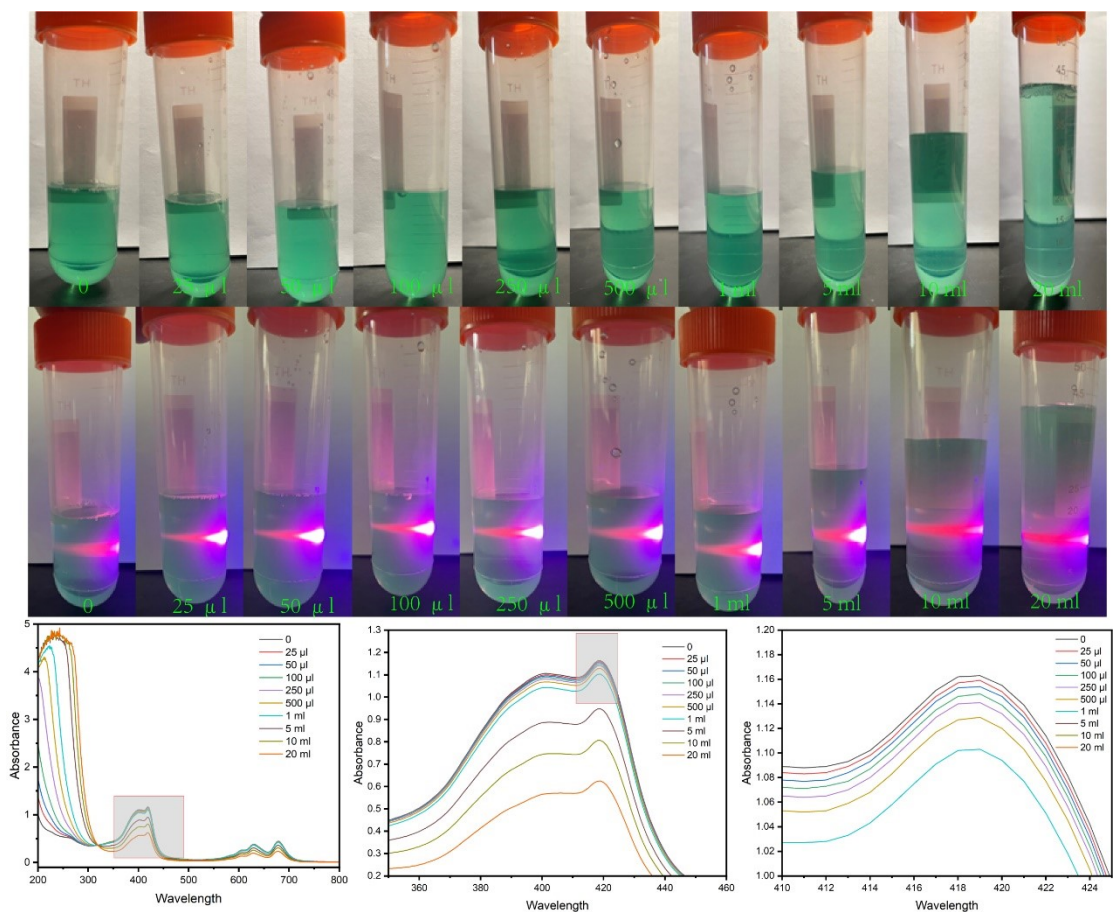


Figure S6 The apparent digital images, the sample images excited by 405nm laser, and UV-vis after adding different volumes of 5w% H₂O₂ solutions

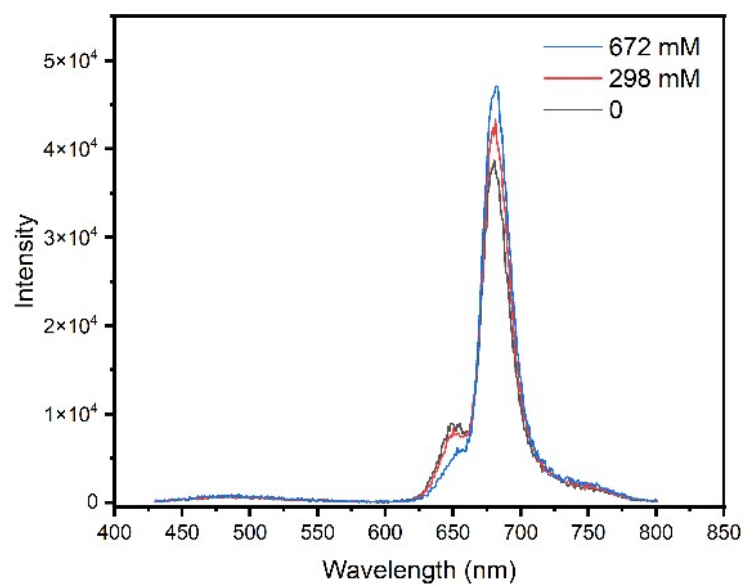


Figure S7 PL spectra of R-CD in H₂O₂ solutions with different concentrations