Supporting Information

Enhancing Luminescence of Carbon Nanodots in Films by Tailoring Functional Groups through Alkylamine-functionalization and Reduction

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Supporting Information contains:

Table S1-S3
Figure S1-S11

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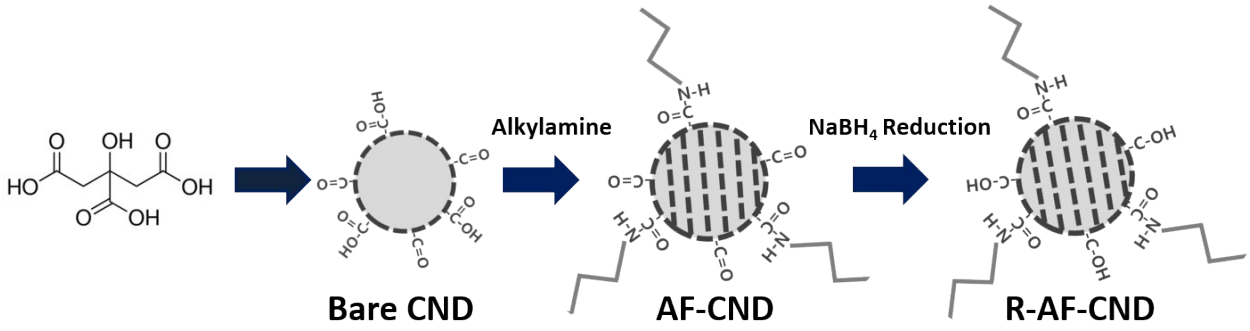

Figure S1. Schematics for the chemical structure of CNDs after alkylamine-functionalization and reduction.

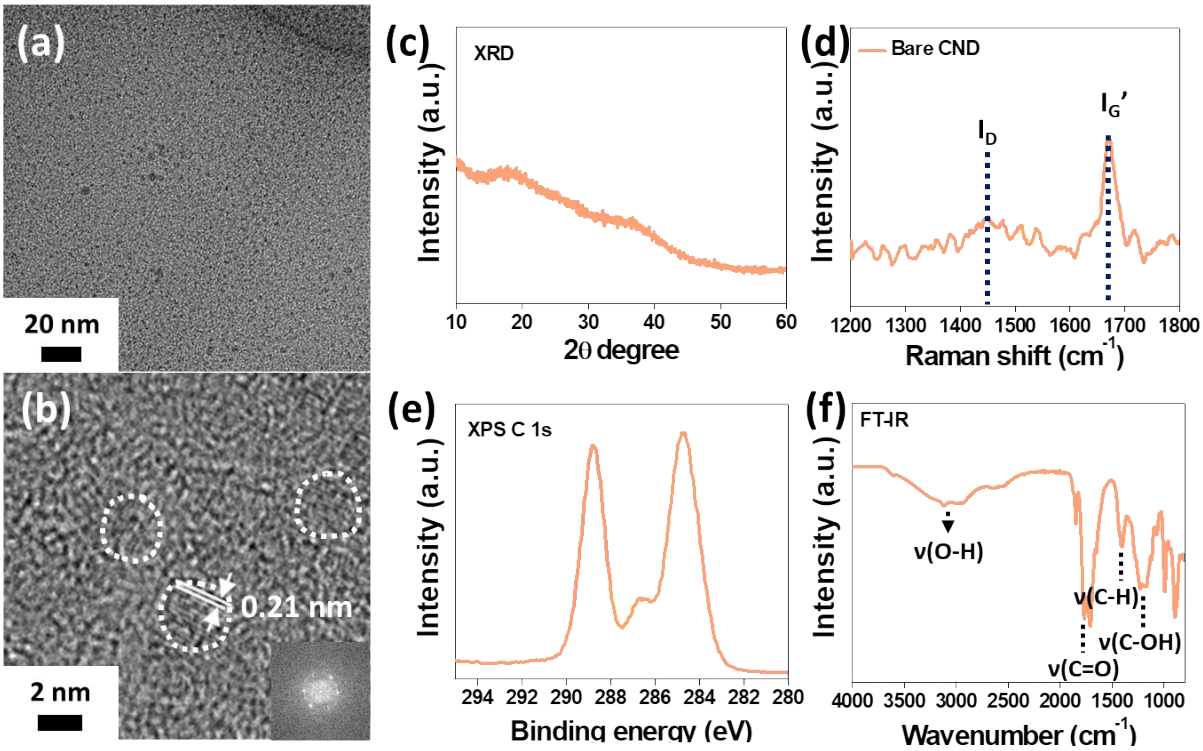

Figure S2. (a, b) HR-TEM image of bare CNDs. The bare CND showed lattice parameter of 0.21 nm corresponding to (100) inter-planar spacing (the inset shows a FFT image). (c) XRD pattern, (d) Raman spectrum with peaks assigned to the corresponding the D and G band, (e) XPS C 1s spectrum, and (f) FT-IR spectrum of bare CNDs with peaks assigned to its corresponding bonds.

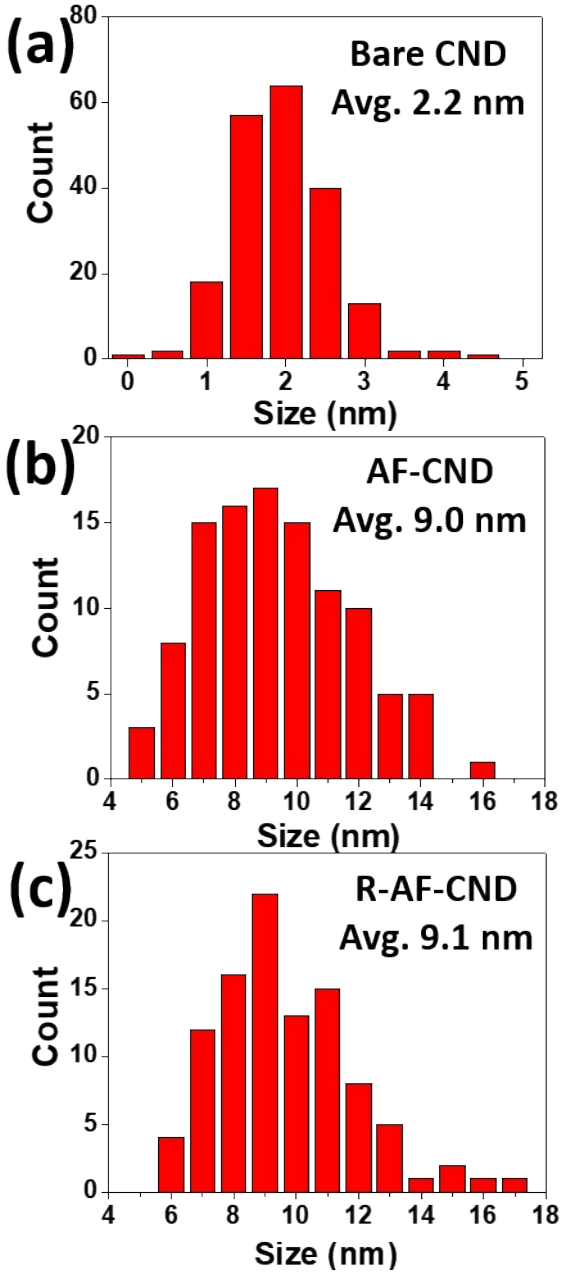

Figure S3. Size histograms of (a) bare CNDs, (b) alkyl chain-functionalized CNDs (AF-CNDs), and (c) reduced AF-CND (R-AF-CND).

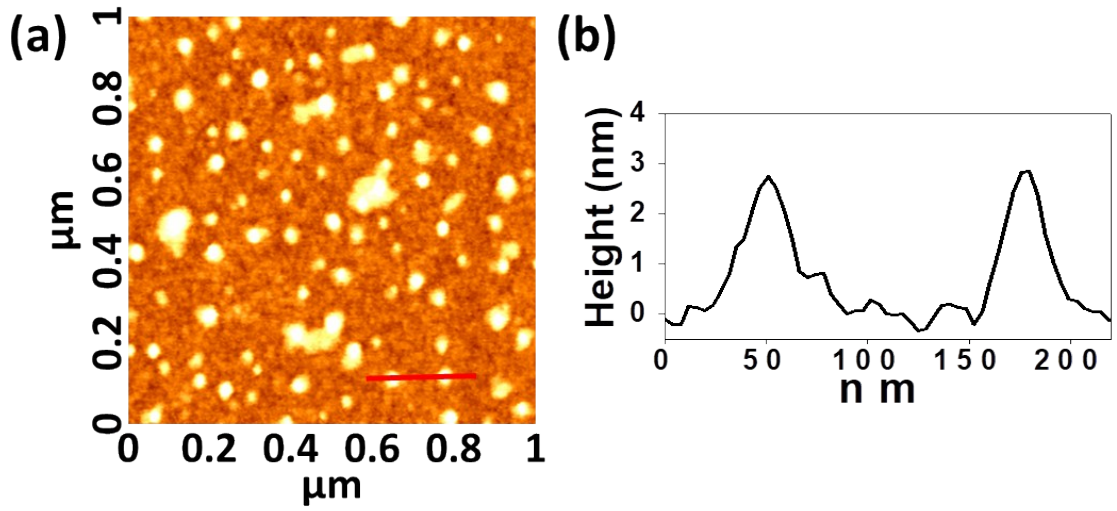

Figure S4. (a) AFM image and (b) a line profile (red line in (a)) of R-AF-CNDs.

Table S1. PL decay times (τ_1, τ_2) and average lifetimes (T_{avg}) estimated from the PL decay curves in Figure 2c[a,b] (excitation at 375 nm)

Sample	Det. Wav. (nm)	T_{avg} (ns)	τ_1 (B1)	f_1 (%)	τ_2 (B2)	f_2 (%)	A	χ^2
Bare CNDs in ethanol	461	4.69	1.163 ns (5296.134)	32.2	6.361 ns (2037.265)	67.8	0.448	1.191
AF-CNDs in hexane	450	6.22	2.452 ns (6264.932)	34.1	8.165 ns (3634.328)	65.9	0.719	1.242
R-AF-CNDs in hexane	445	8.88	3.197 ns (4394.988)	20.2	10.32 ns (5389.898)	79.8	1.341	1.186

[a] Intensity = $A+B1\exp(-t/\tau_1)+B2\exp(-t/\tau_2)$

[b] $T_{avg} = f_1 \tau_1 + f_2 \tau_2$

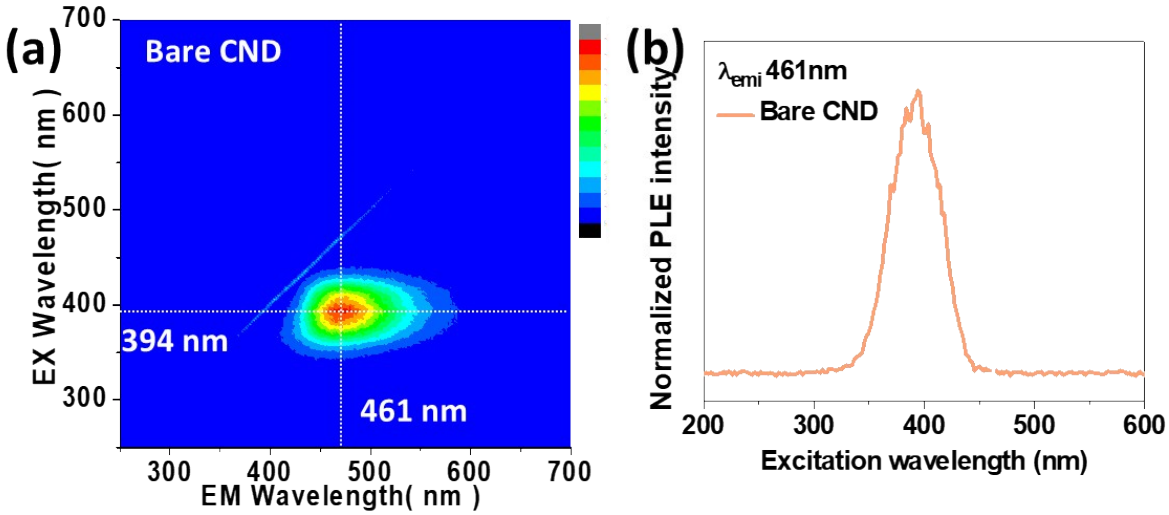

Figure S5. (a) Photoluminescence map and (b) photoluminescence excitation (PLE) spectrum for bare CNDs.

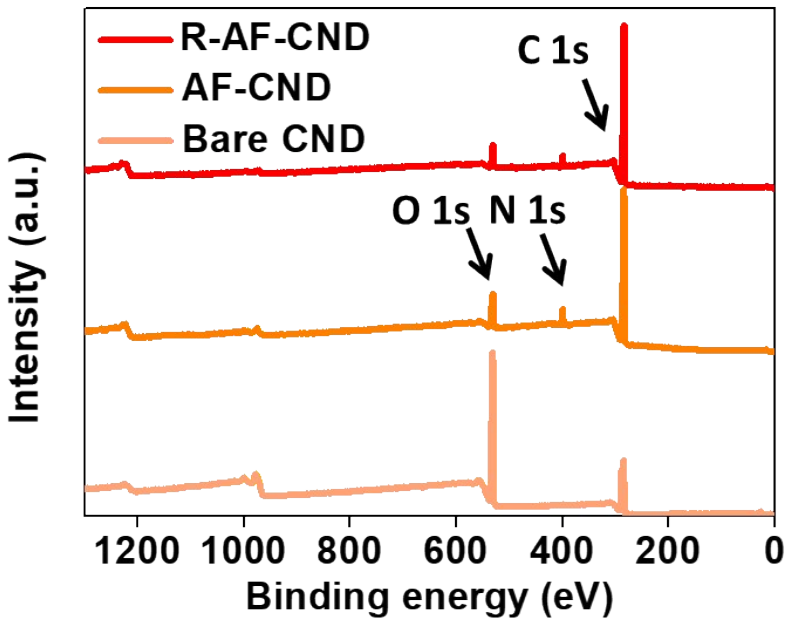

Figure S6. XPS survey spectra of bare CNDs, AF-CNDs, and R-AF-CNDs.

Table S2. The changes in C, N, O contents in bare CNDs, AF-CNDs, and R-AF-CNDs determined by XPS survey scan

Sample	C (atomic%)	N (atomic%)	O (atomic%)	Others (atomic%)
Bare CNDs	55.6	-	44.4	-
AF-CNDs	85.2	5.2	9.5	-
R-AF-CNDs	88.9	3.8	6.0	1.3

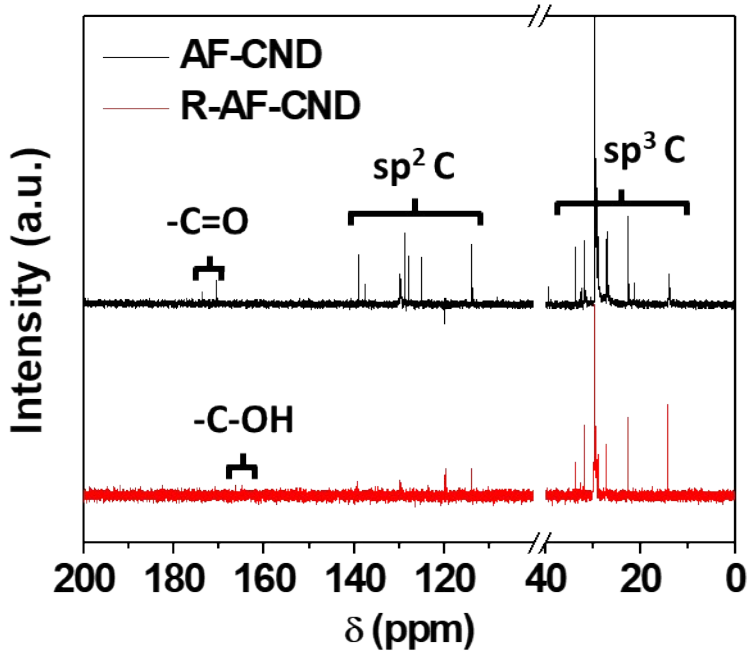

Figure S7. ^{13}C NMR results of AF-CNDs and R-AF-CNDs.

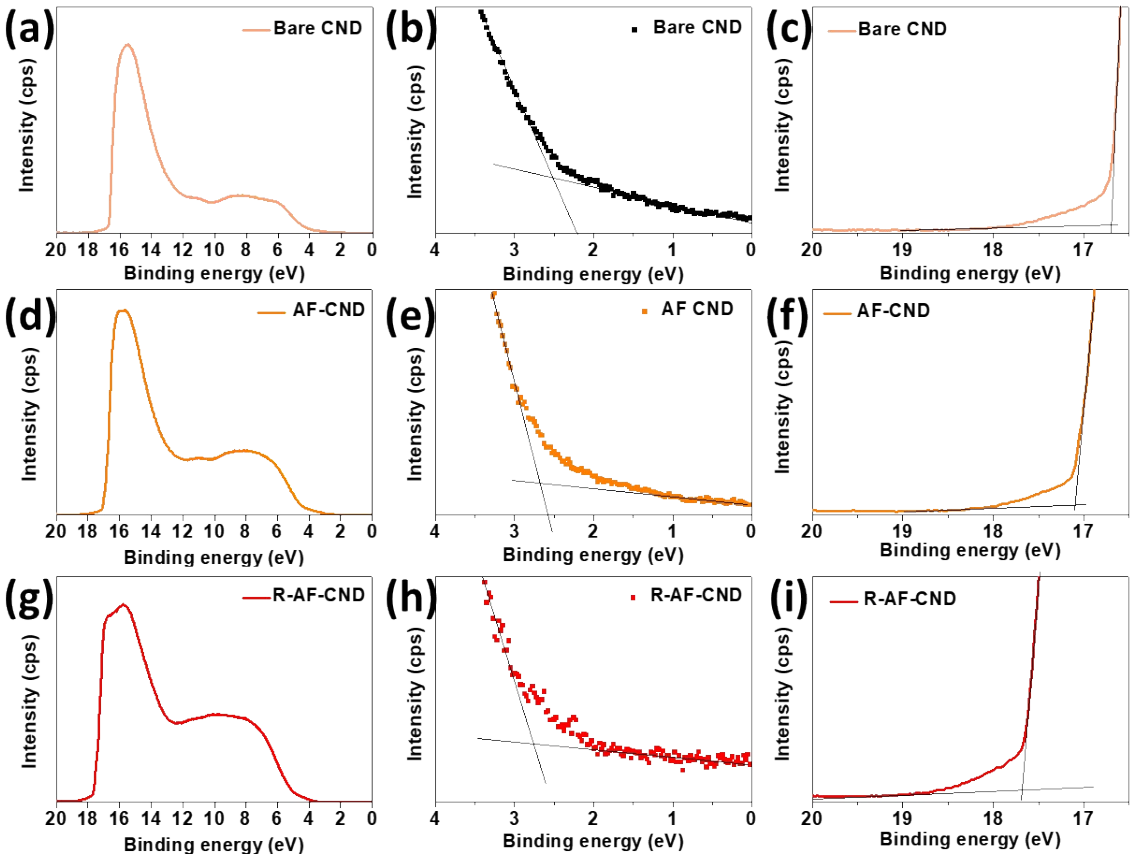

Figure S8. UPS data of (a-c) bare CNDs, (d-f) AF-CNDs, and (g-i) R-AF-CNDs

Table S3. PLE onset wavelength, energy band gap, HOMO, and LUMO level of bare CNDs, AF-CNDs, and R-AF-CNDs[a]

Sample	$\lambda_{ex,\ onset}$[b] (nm)	E_g[c] (eV)	E_{cutoff}[d] (eV)	E_{Fermi}[d] (eV)	HOMO[e] (eV)	LUMO[f] (eV)
Bare CNDs	394	3.15	16.68	2.53	7.05	3.9
AF-CNDs	394	3.15	17.07	2.68	6.81	3.6
R-AF-CNDs	412	3.01	17.66	2.75	6.29	3.28

[a] The incident photon energy from He I source is 21.2 eV and the -9 V bias was applied to make a clear boundary in the E_{cutoff} region.

[b] The onset wavelength of photoluminescence excitation ($\lambda_{ex,\ onset}$) were obtained from Figure 3 and Figure S5.

[c] The optical band gap (E_g) was obtained by a following equation;

$$E_g = 1240/\ \lambda_{ex,\ onset}$$

[d] The E_{cutoff} and E_{Fermi} were extracted by the intersection between the base line and a linear fit from near Fermi energy region (Figure S8 (b,e,h)) and secondary electron cut-off region (Figure S8 (c,f,i)).

[e] The HOMO level was calculated by a following equation;

$$\text{HOMO (eV)} = h\nu \text{ (incident photon energy, 21.1eV)} - E_{cutoff} + E_{Fermi}$$

[f] The LUMO level was calculated by a following equation;

$$\text{LUMO (eV)} = \text{HOMO (eV)} - E_g$$

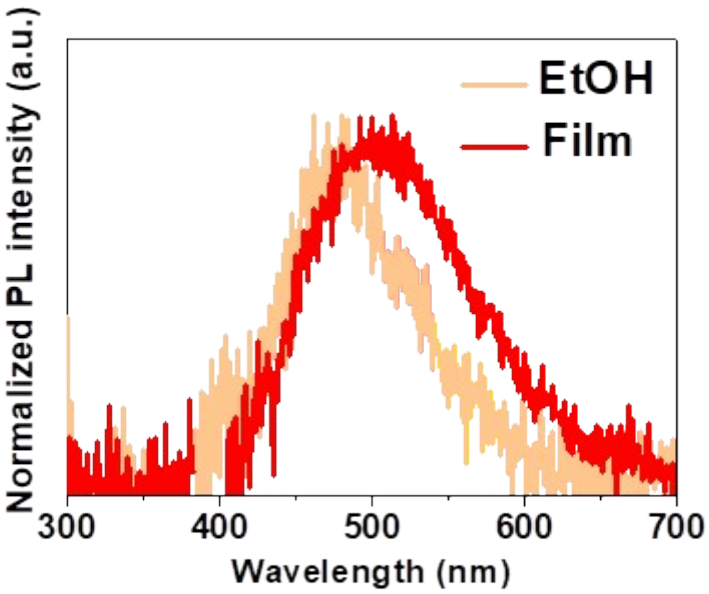

Figure S9. Normalized PL spectra (excitation at 390 nm) of bare CNDs in a solution (ethanol) and a film. The PLQY was 5.9% for the solution and 3.9% for the film. FWHM was 91 nm for the solution and 124 nm for the film.

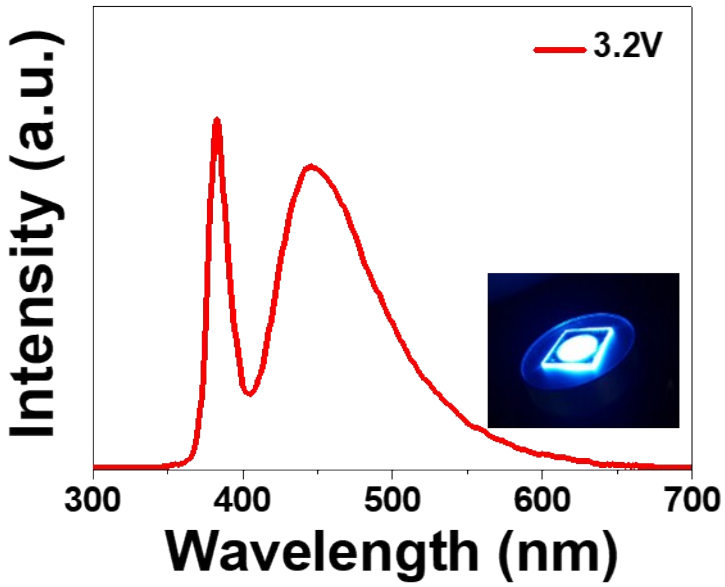

Figure S10. Photoluminescence spectrum of blue LED using R-AF-CNDs with 385 nm UV chip. The inset photograph shows R-AF-CND film under UV light.

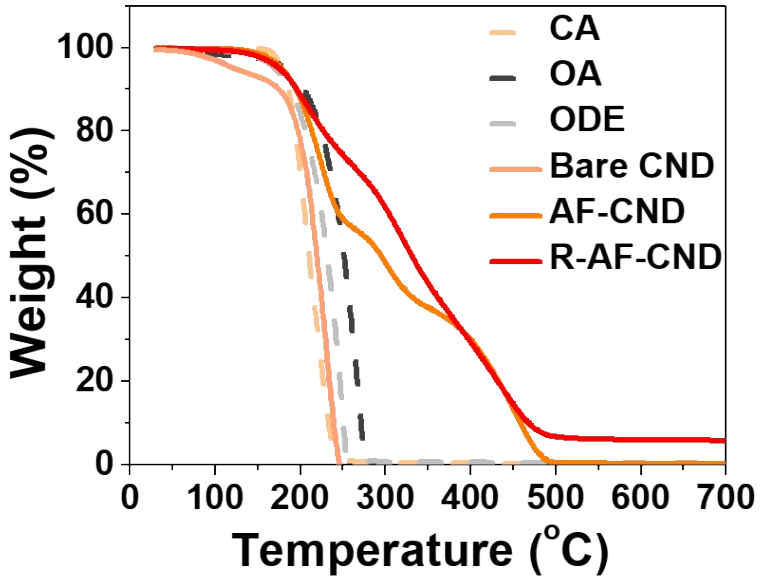

Figure S11. TGA results of the CNDs. CA indicates citric acid, OA indicates oleylamine, and ODE indicates octadecene.