Electronic Supporting Material

Lignin-Derived Red-emitting Carbon Dots for Colorimetric and Sensitive Fluorometric Detection of Water in Organic Solvents

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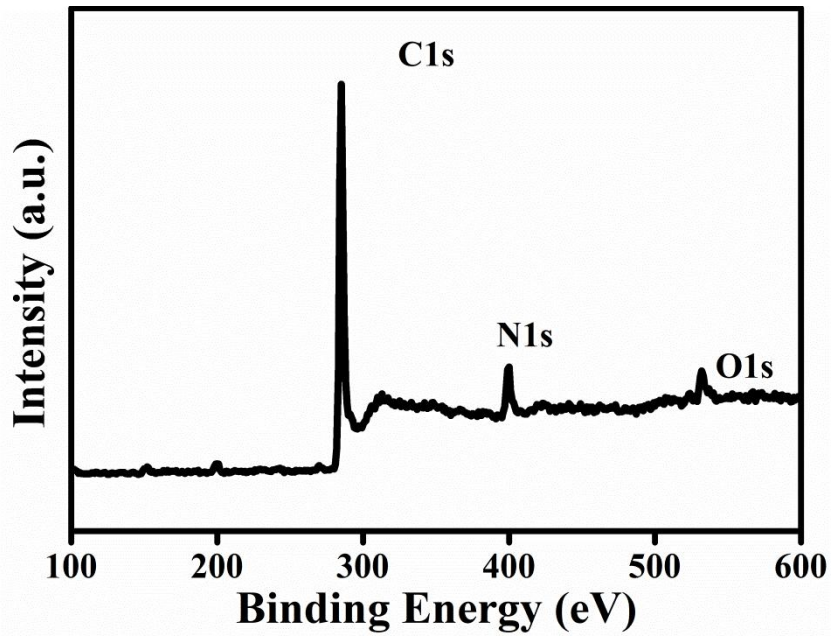

Fig. S1. XPS spectra of the RCDs

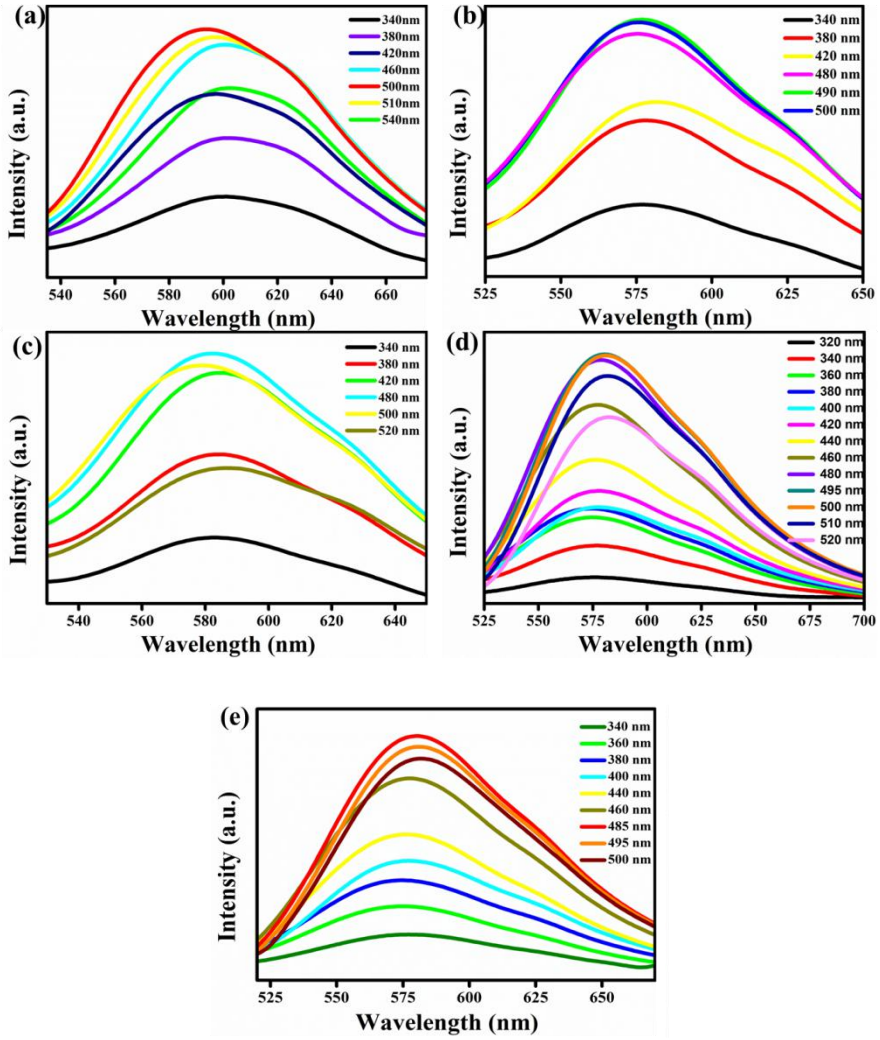

Fig. S2. Excitation-independent PL spectra of RCDs in different organic solvents (a) Ethanol, (b) DMF, (c) DMSO, (d) THF, (e) Ether.

Quantum yield (QY) measurement

The quantum yield (QY) of the RCDs was calculated according to a widely accepted formula, [1]

$\varphi_x = \varphi_{st} (K_x / K_{st}) (\eta_x / \eta_{st})^2$

Where φ is the QY, K is on behalf of the slope and η is the refractive index. The subscript "x" and "st" reveal sample and standard, respectively.

Refractive index of different solvents

EtOH	Water	DMSO	DMF	THF	Acetone	Ether	Chloroform
1.361	1.333	1.478	1.431	1.407	1.359	1.352	1.446

Table S1. Quantum yields (QY) in various solvents/water under excitation of 365 nm and maximum excitation wavelength

		$Slope_x(10^5)$	$Slope_{st}(10^5)$	QY(%)		$Slope_s(10^5)$		$Slope_r(10^5)$	QY(%)
Ethanol	365 nm	0.302	1.12	15.03	Water	365 nm	0.0967	1.12	4.62
	500 nm	0.558	4.37	7.14		480 nm	0.0938	1.49	3.37
DMSO	365 nm	0.635	1.12	37.29	DMF	365 nm	0.319	1.12	17.53
	480 nm	1.53	1.49	67.57		490 nm	0.854	2.69	19.61
THF	365 nm	0.519	1.12	27.65	Acetone	365 nm	0.736	1.12	36.55
	500 nm	0.868	4.37	11.88		480 nm	1.99	1.49	74.46
Ether	365 nm	1.0	1.12	47.31					
	485 nm	2.52	2.02	68.89					

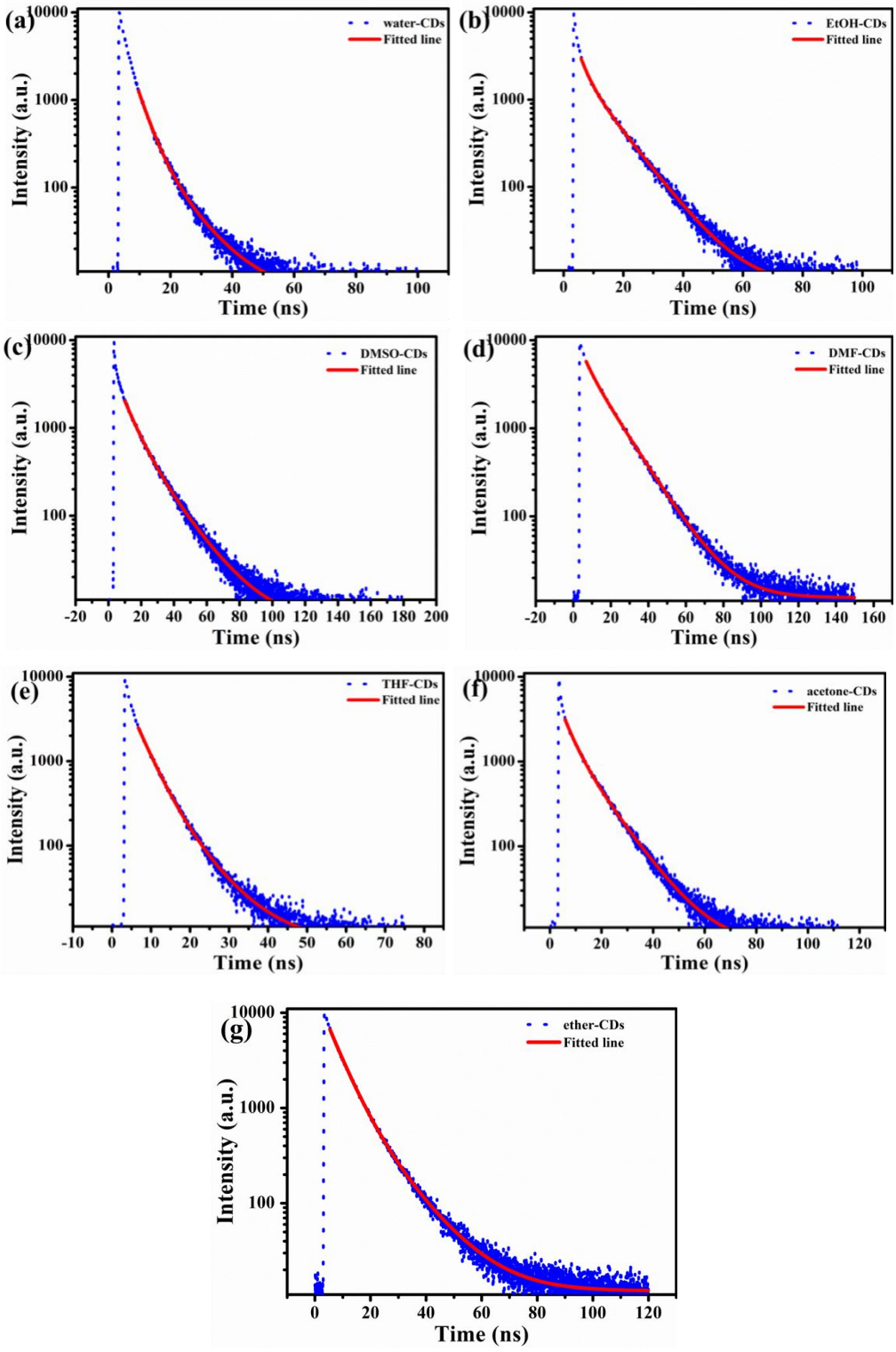

Fig. S3. PL decay spectra of different solvents under excitation of 375 nm, water (a), ethanol (b), DMSO (c), DMF (d), THF (e), acetone (f), ether (g).

Table S2. The fluorescence lifetimes of CDs in different solvents (375 nm excitation)

	λ_{ex}(nm)	λ_{em}(nm)	Bi_1(%)	τ_1(ns)	Bi_2(%)	τ_2(ns)	τ_{avg}(ns)	χ^2
Ethanol	375	599	85.3	9.777	14.7	2.635	8.721	1.303
Water	375	564	44.4	9.870	55.6	3.586	6.396	1.309
DMSO	375	579	59.7	17.330	40.3	7.590	13.401	1.353
DMF	375	439	79.8	12.999	20.2	4.340	12.325	1.136
THF	375	574	34.3	8.350	65.7	3.748	5.323	1.246
Acetone	375	559	73.4	10.350	26.6	3.938	8.643	1.273
Ether	375	574	37.7	12.450	62.3	5.477	8.099	1.190

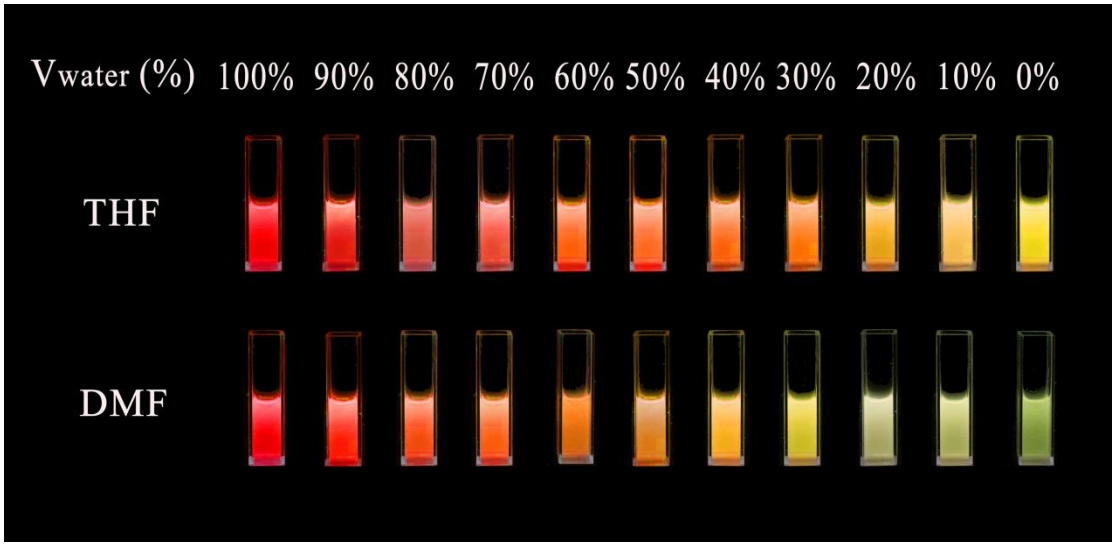

Fig. S4. Colorimetric detection of water contents in various organic solvents via RCDs.

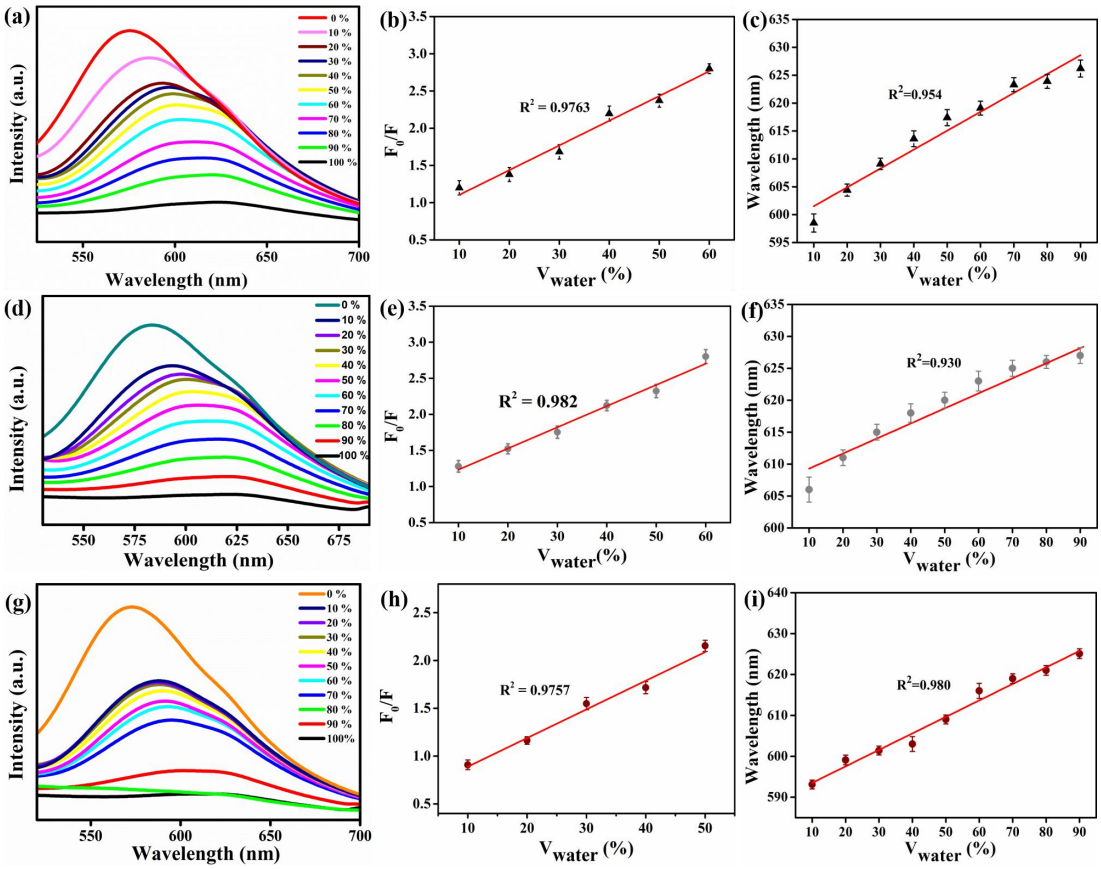

Fig. S5. Fluorescence spectra of RCDs for sensing water content from 0-100% in various organic solvents, DMF (a), DMSO (d), THF (g); Relationships of relative PL intensity and water content of 10-60% in DMF (b), DMSO (e) and 10-50% in THF (h); Relationships of PL peaks position and water content of 10-90% in DMF (c), DMSO (f), THF (i).

Table S3. Linear equations, LODs and linear range for water sensing via RCDs

Solvent	Function	R^2	Linear range (%)	LOD (%)
Ethanol	$F_0/F=0.0193[H_2O]+1.0037$	0.983	10 ~ 60	0.360
	$\lambda=0.2291[water]+608.23$	0.980	10 ~ 90	3.10
DMSO	$F_0/F=0.0268[H_2O]+0.9974$	0.982	10 ~ 60	0.160
	$\lambda=0.2358[water]+606.93$	0.930	10 ~ 90	1.570
DMF	$F_0/F=0.0287[H_2O]+0.9180$	0.976	10 ~ 60	0.159
	$\lambda=0.3404[water]+598.03$	0.954	10 ~ 90	1.432
THF	$F_0/F=0.0245[H_2O]+0.9023$	0.976	10 ~ 50	0.338
	$\lambda=0.4032[water]+589.48$	0.980	10 ~ 90	2.764
Acetone	$F_0/F=0.0328[H_2O]+1.0339$	0.971	10 ~ 60	0.082
	$\lambda=0.3667[water]+593.11$	0.992	10 ~ 90	0.73
Ether	$F_0/F=0.0284[H_2O]+1.0505$	0.961	0~8	0.122

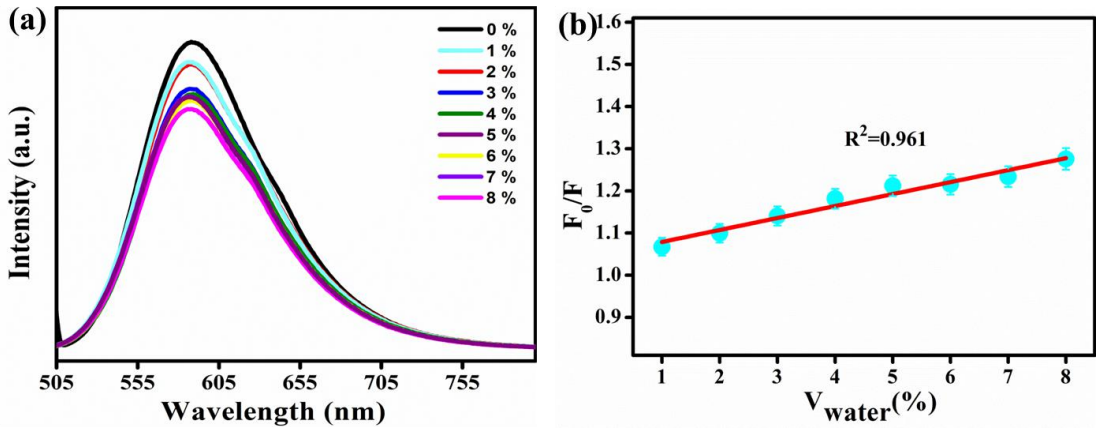

Fig. S6. (a) the fluorescence spectra of RCDs for sensing water content in ether, (b) Relationships of relative PL intensity and water content of 1-8% in ether.

Table S4. Summary of water sensing via various methods

Raw material	Detection method	Linear function	Linear detection range	LOD	Number of organic solvents	Refs
OPD	Fluorescence	none	50-90 %	0.19 %	5	2
OPD	Fluorescence	none	0-70 %	0.03 %	1	3
Resorcinol	Fluorescence	none	0-1 %	0.006%	5	4
1H-Imidazole-carboxylic	Fluorescence	none	0-20 %	0.1 %	3	5
Lignin PPD	Fluorescence and Colorimetric	relative	10-90 %	0.082%	6	This work

References:

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