A Coumarin-Hemicyanine Near-Infrared Dye with a Large Stokes Shift for the Fluorescence Detection of Cyanide and Naked-Eye Recognition

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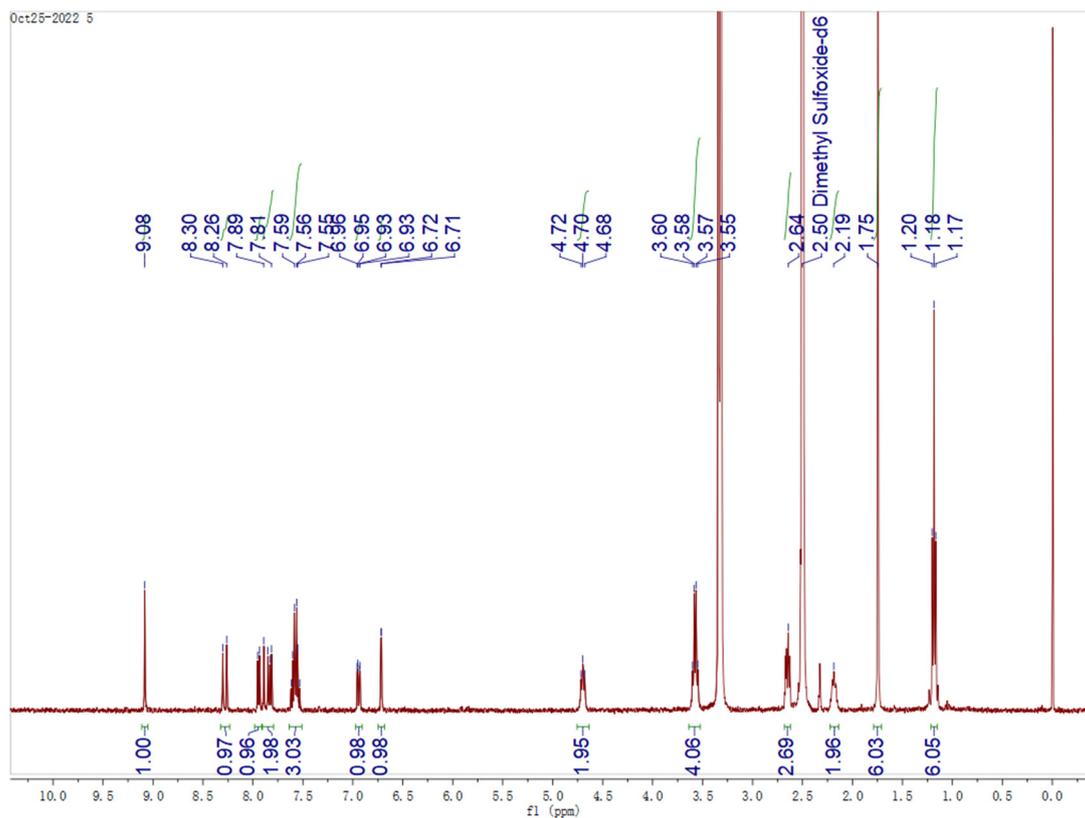
Figure S1. ¹H NMR spectrum of probe W
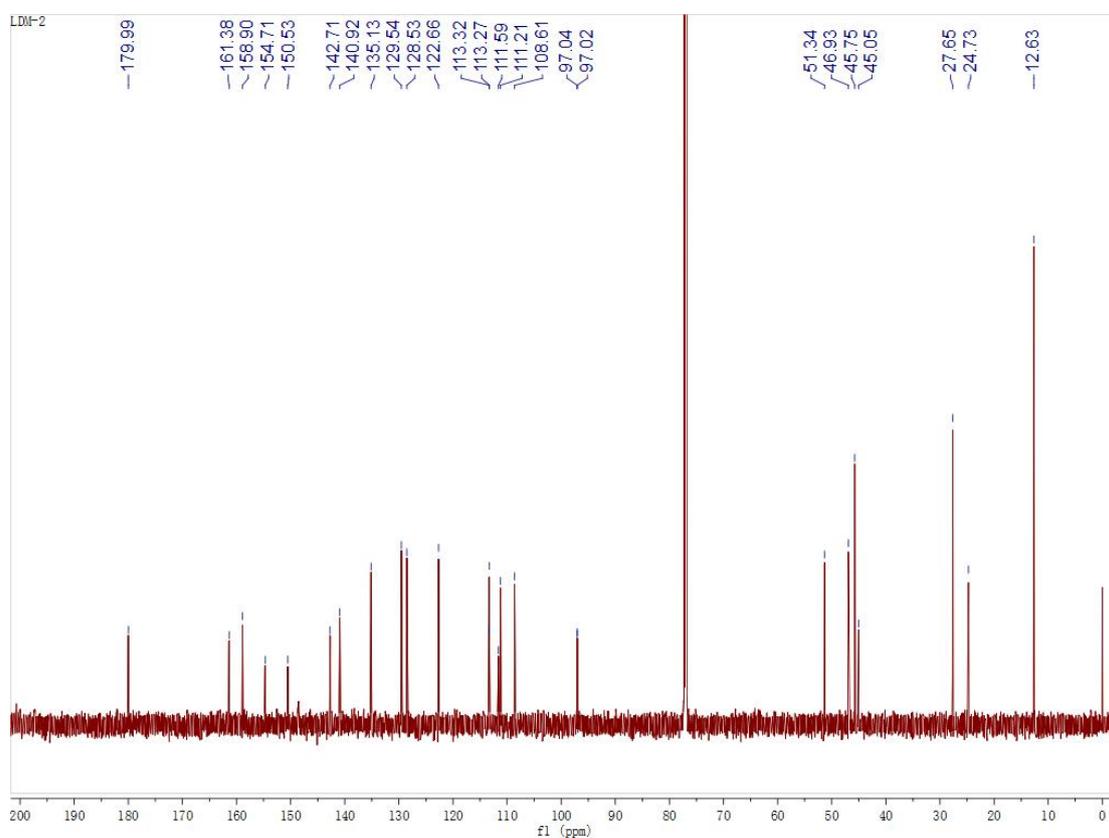

Figure S2. ¹³C NMR spectrum of probe W
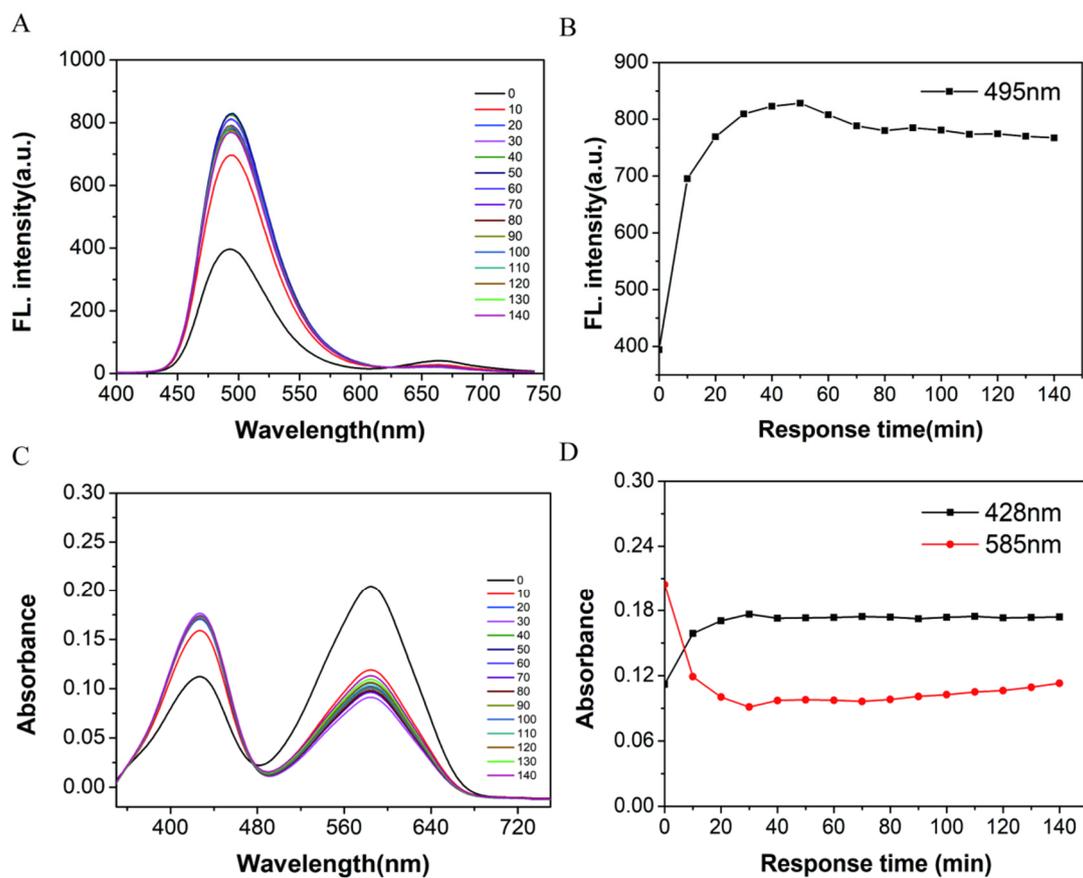
Figure S3. Time-varying fluorescence spectra (A) of probe W-CN⁻solution in dimethyl sulfoxide/water ($V_{DMSO}:V_{H2O}$=1:4, 1.00×10^{-2}mol/L PBS buffer) detection system; changes in fluorescence intensities of probe W-CN⁻solution over time at the maximum emission at λ_{em}=495nm, slit. 5/5nm, voltage: 700V (B); UV-Vis absorption spectra (C) and the effect of time-dependent UV-visible absorbance of probe W-CN⁻solution at λ=428/585nm (D).

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Table S1. Summary of crystal data for W

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Parameter	W
Empirical formula	$C_{28}H_{32}N_2O_5S$
Formula weight [g mol^{-1}]	508.61
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	16.317(3)
b [Å]	7.8841(17)
c [Å]	20.827(4)
α	90.00°
β	104.707(9)
γ	90.00°
Volume [Å^3]	2591.6(9)
Z	4
Density, calcd [gm^{-3}]	1.304
Temperature [K]	300(2)
Unique reflns	2463
Obsd reflns	4564
Parameters	330
R_{int}	0.0774
$R[I>2\sigma(I)]^a$	0.0745
W[all data]R^b	0.1679
GOF on F^2	1.060

Table S2. Hydrogen-bonding geometries for compound W

D−H⋯A	d(D⋯H)/nm	d(H⋯A)/nm	d(D⋯A)/nm	∠D−H⋯A/ (°)
C(10)-H(10B)-F(3) [i]	0.096	0.254	0.329 9(4)	137
C(10)-H(10B)-F(4) [i]	0.096	0.243	0.337 8(4)	170
C(3)-H(3)-F(1) [ii]	0.093	0.254	0.343 0(4)	161
C(10)-H(10C)-O(2) [iii]	0.096	0.257	0.337 9(4)	141
C(18)-H(18A)-F(4) [iii]	0.097	0.251	0.331 3(4)	140
C(19)-H(19B)-F(2)	0.096	0.250	0.338 6(4)	153
C25—H25B⋯O4 [i]	0.97	2.40	3.242 (6)	144.6
C24—H24⋯O4 [i]	0.93	2.40	3.306 (5)	164.7
C14—H14⋯O2 [ii]	0.93	2.43	3.348 (6)	171.0
C3—H3A⋯O2 [ii]	0.97	2.62	3.458 (6)	145.0
C1—H1B⋯O2 [ii]	0.97	2.48	3.347 (6)	149.4

Symmetry codes: i −x+1, −y, −z+1; ii x−1, y, z; iii x, −y+1/2, z+1

Table S3. Comparison data with reported CN⁻ sensors

Structure	Fluorescence	solvent	Detection limit
Our work	Turn-on	DMSO/ H_2O (1:4)	0.24 μM/ 0.13 μM
Probe R [2]	Turn-on	DMSO/ H_2O (2:8)	0.96 μM
Probe 1 [3]	Turn-on	DMF/H_2O (6:4)	0.23 μM
Q1-3 [4]	Turn-on	DMSO/ H_2O (1:9)	0.81 μM
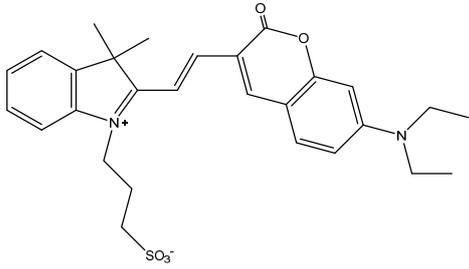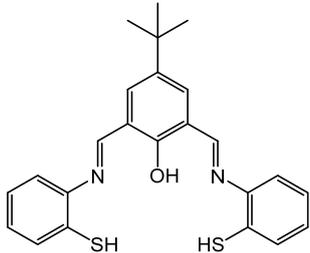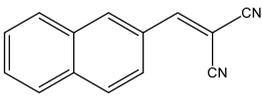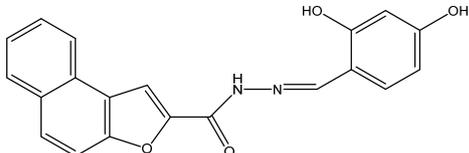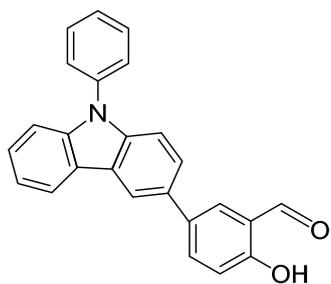
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CPHB [5]	Turn-on	THF/ H₂O (1:19)	0.249 μM
YS [6]	Turn-on	DMSO/ H₂O (3:7)	0.17 μM
L1 [7]	Turn-on	DMSO/ H₂O (4:1)	0.947 μM
AZQ [8]	Turn-on	EtOH/ H₂O (1:1)	2.6μM
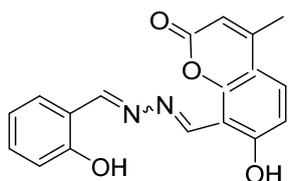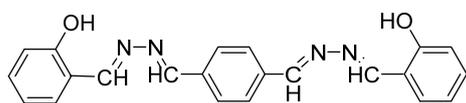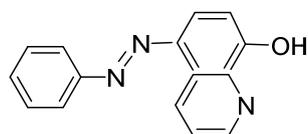
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