Supporting Information for

Efficient synthesis of diethyl benzo[c]cinoline-3,8-dicarboxylate for fluorescent quenching materials

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Supplementary Index

1. Crystal data

Table S1. Selected bond lengths (Å) and angles (°) for the Intermediate **D**

Intermediate **D**			
O(4)-C(9)	1.191(3)	O(2AA)-C(1AA)	1.198(4)
O(0AA)-C(9)	1.321(3)	O(0AA)-C(10)	1.452(3)
O(1AA)-C(1AA)	1.318(4)	O(1AA)-C(19)	1.464(4)
C(14)-C(15)	1.437(3)	C(14)-C(6)	1.393(3)
C(14)-C(13)	1.398(3)	C(15)-C(4)	1.404(3)
C(15)-C(16)	1.390(4)	C(6)-C(7)	1.390(4)
C(6)-N(1)	1.420(3)	C(8)-C(7)	1.368(3)
C(8)-C(12)	1.393(3)	C(8)-C(9)	1.484(4)
C(7)-H(7)	0.9300	C(4)-C(0AA)	1.397(4)
C(4)-N(3)	1.382(3)	C(12)-H(12)	0.9300
C(12)-C(13)	1.369(4)	C(13)-H(13)	0.9300
C(16)-H(16)	0.9300	C(16)-C(17)	1.365(4)
C(0AA)-H(0AA)	0.9300	C(0AA)-C(2AA)	1.370(4)
C(17)-H(17)	0.9300	C(17)-C(2AA)	1.400(4)
C(2AA)-C(1AA)	1.483(4)	C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700	C(10)-C(11)	1.478(5)
C(11)-H(11A)	0.9600	C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600	C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700	C(19)-C(20)	1.360(6)
C(20)-H(20A)	0.9600	C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600	N(1)-O(5)	1.272(3)
N(1)-N(3)	1.300(3)	N(3)-O(5A)	1.130(15)
C(9)-O(0AA)-C(10)	118.0(2)	C(1AA)-O(1AA)-C(19)	114.9(3)
C(6)-C(14)-C(15)	118.5(2)	C(6)-C(14)-C(13)	117.4(2)
C(13)-C(14)-C(15)	124.1(2)	C(4)-C(15)-C(14)	116.5(2)
C(16)-C(15)-C(14)	124.9(2)	C(16)-C(15)-C(4)	118.6(2)
C(14)-C(6)-N(1)	120.1(2)	C(7)-C(6)-C(14)	122.1(2)
C(7)-C(6)-N(1)	117.8(2)	C(7)-C(8)-C(12)	119.5(2)
C(7)-C(8)-C(9)	118.5(2)	C(12)-C(8)-C(9)	122.0(2)
C(6)-C(7)-H(7)	120.3	C(8)-C(7)-C(6)	119.3(2)
C(8)-C(7)-H(7)	120.3	C(0AA)-C(4)-C(15)	120.3(2)
N(3)-C(4)-C(15)	123.6(2)	N(3)-C(4)-C(0AA)	116.1(2)
C(8)-C(12)-H(12)	119.4	C(13)-C(12)-C(8)	121.2(2)
C(13)-C(12)-H(12)	119.4	C(14)-C(13)-H(13)	119.7
C(12)-C(13)-C(14)	120.5(2)	C(12)-C(13)-H(13)	119.7
C(15)-C(16)-H(16)	119.5	C(17)-C(16)-C(15)	121.0(3)
C(17)-C(16)-H(16)	119.5	C(4)-C(0AA)-H(0AA)	120.1
C(2AA)-C(0AA)-C(4)	119.9(3)	C(2AA)-C(0AA)-H(0AA)	120.1

C(16)-C(17)-H(17)	119.8	C(16)-C(17)-C(2AA)	120.4(3)
C(2AA)-C(17)-H(17)	119.8	C(0AA)-C(2AA)-C(17)	119.9(3)
C(0AA)-C(2AA)-C(1AA)	122.3(3)	C(17)-C(2AA)-C(1AA)	117.8(3)
O(4)-C(9)-O(0AA)	124.2(3)	O(4)-C(9)-C(8)	124.1(3)
O(0AA)-C(9)-C(8)	111.7(2)	O(2AA)-C(1AA)-O(1AA)	123.1(3)
O(2AA)-C(1AA)-C(2AA)	124.4(3)	O(1AA)-C(1AA)-C(2AA)	112.5(3)
O(0AA)-C(10)-H(10A)	110.3	O(0AA)-C(10)-H(10B)	110.3
O(0AA)-C(10)-C(11)	106.9(3)	H(10A)-C(10)-H(10B)	108.6
C(11)-C(10)-H(10A)	110.3	C(11)-C(10)-H(10B)	110.3
C(10)-C(11)-H(11A)	109.5	C(10)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5	H(11A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
O(1AA)-C(19)-H(19A)	109.6	O(1AA)-C(19)-H(19B)	109.6
H(19A)-C(19)-H(19B)	108.1	C(20)-C(19)-O(1AA)	110.3(4)
C(20)-C(19)-H(19A)	109.6	C(20)-C(19)-H(19B)	109.6
C(19)-C(20)-H(20A)	109.5	C(19)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
O(5)-N(1)-C(6)	118.5(2)	O(5)-N(1)-N(3)	119.2(2)
N(3)-N(1)-C(6)	122.3(2)	N(1)-N(3)-C(4)	119.0(2)
O(5A)-N(3)-C(4)	108.5(8)	O(5A)-N(3)-N(1)	132.1(8)

Table S2. Selected bond lengths (Å) and angles (°) for the compound **2**

Compound **2**			
O(1)-C(7)	1.328(3)	O(1)-C(8)	1.446(3)
O(2)-C(7)	1.200(3)	N(1)-N(2)	1.322(6)
N(1)-C(3)	1.224(5)	N(2)-C(5)#1	1.312(5)
C(1)-C(2)	1.390(3)	C(1)-C(6)	1.388(4)
C(1)-C(7)	1.476(4)	C(2)-H(2)	0.9300
C(2)-C(3)	1.373(4)	C(3)-H(3)	0.9300
C(3)-C(4)	1.397(4)	C(4)-C(4)#1	1.413(6)
C(4)-C(5)	1.385(5)	C(5)-N(2)#1	1.312(5)
C(5)-H(5)	0.9300	C(5)-C(6)	1.374(4)
C(6)-H(6)	0.9300	C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700	C(8)-C(9)	1.469(4)
C(9)-H(9A)	0.9600	C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600		
C(7)-O(1)-C(8)	116.7(2)	C(3)-N(1)-N(2)	125.7(4)
C(5)#1-N(2)-N(1)	129.1(4)	C(2)-C(1)-C(7)	122.1(2)
C(6)-C(1)-C(2)	119.0(2)	C(6)-C(1)-C(7)	118.9(2)
C(1)-C(2)-H(2)	119.9	C(3)-C(2)-C(1)	120.3(3)
C(3)-C(2)-H(2)	119.9	N(1)-C(3)-C(2)	125.6(4)
N(1)-C(3)-C(4)	112.9(3)	C(2)-C(3)-H(3)	119.3
C(2)-C(3)-C(4)	121.5(3)	C(4)-C(3)-H(3)	119.3

C(3)-C(4)-C(4)#1	122.0(5)	C(5)-C(4)-C(3)	117.1(3)
C(5)-C(4)-C(4)#1	120.9(5)	N(2)#1-C(5)-C(4)	109.5(4)
N(2)#1-C(5)-C(6)	128.3(4)	C(4)-C(5)-H(5)	118.9
C(6)-C(5)-C(4)	122.2(3)	C(6)-C(5)-H(5)	118.9
C(1)-C(6)-H(6)	120.1	C(5)-C(6)-C(1)	119.8(3)
C(5)-C(6)-H(6)	120.1	O(1)-C(7)-C(1)	112.1(2)
O(2)-C(7)-O(1)	123.4(3)	O(2)-C(7)-C(1)	124.5(3)
O(1)-C(8)-H(8A)	110.0	O(1)-C(8)-H(8B)	110.0
O(1)-C(8)-C(9)	108.4(2)	H(8A)-C(8)-H(8B)	108.4
C(9)-C(8)-H(8A)	110.0	C(9)-C(8)-H(8A)	110.0
C(8)-C(9)-H(9A)	109.5	C(8)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5	H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5

2. ^{1}H NMR

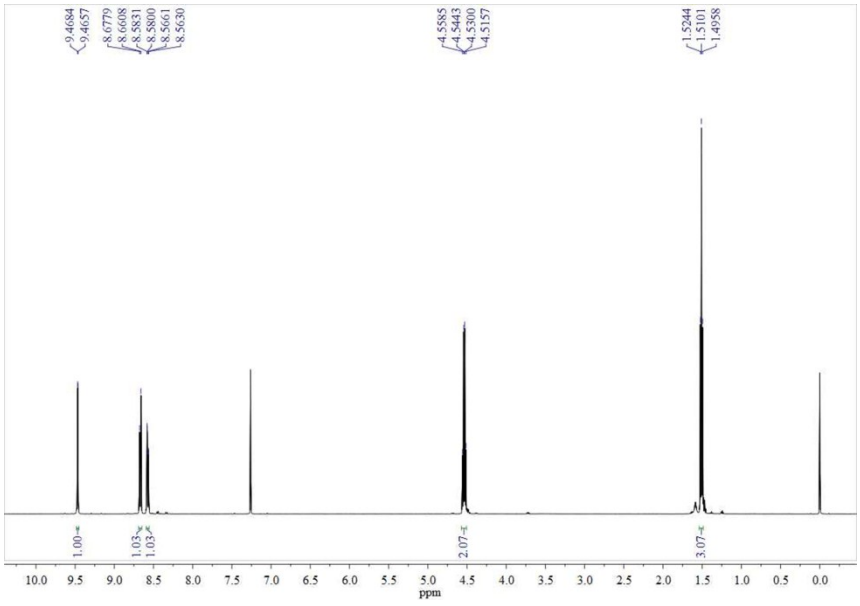


Fig. S1 ^{1}H NMR spectrum of compound **2**

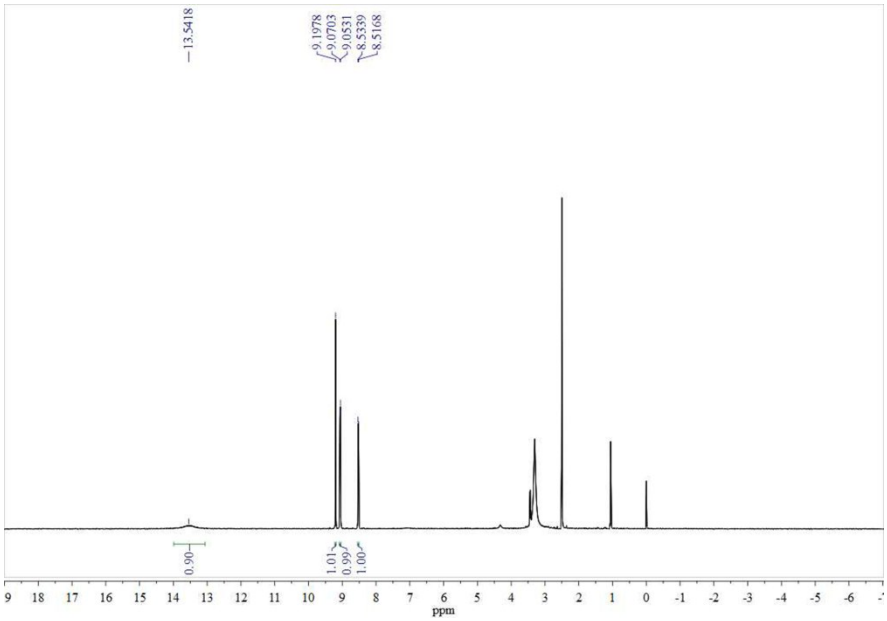


Fig. S2 ^{1}H NMR spectrum of compound **3**

3. ^{13}C NMR

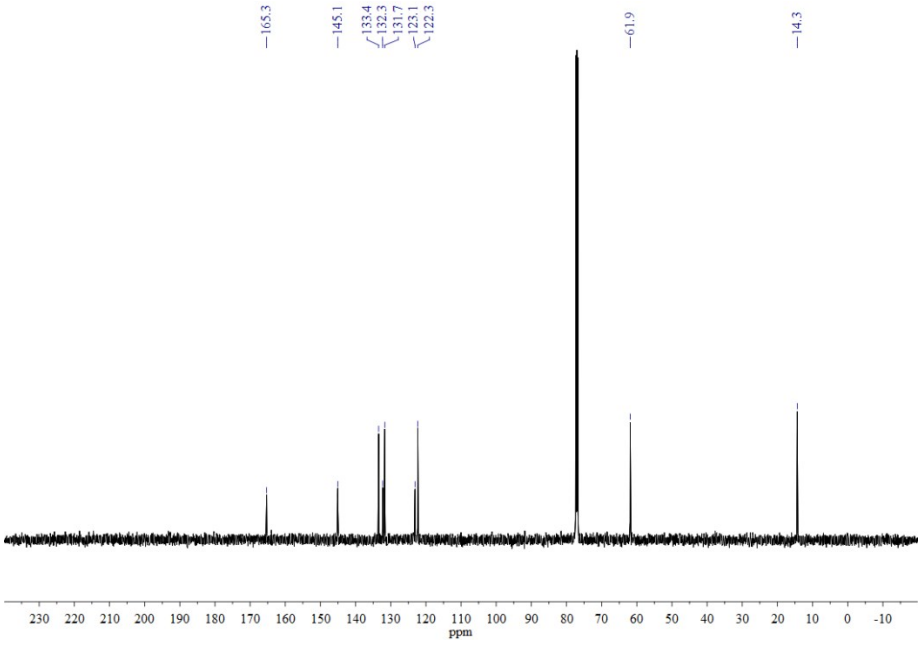


Fig. S3 ^{13}C NMR spectrum of compound **2**

4. MS Spectra

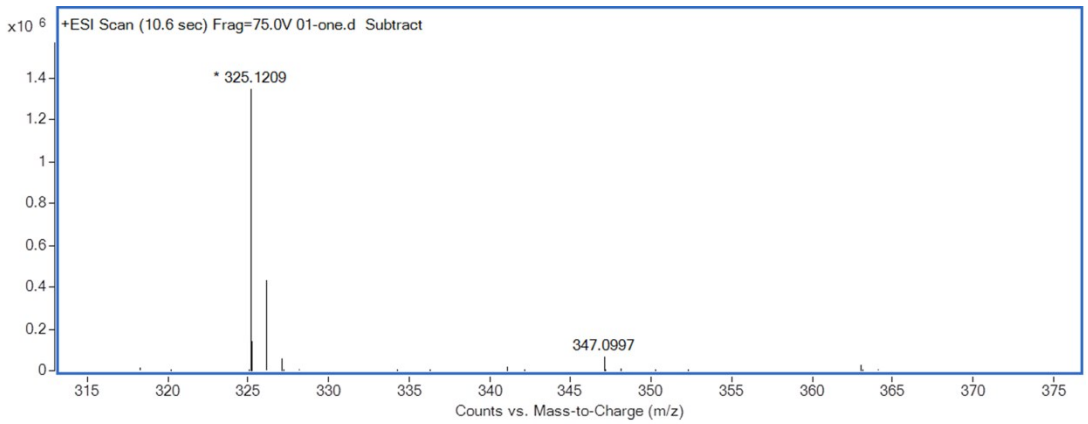


Fig. S4. ESI-MS spectrum of compound **2**

5. PXRD

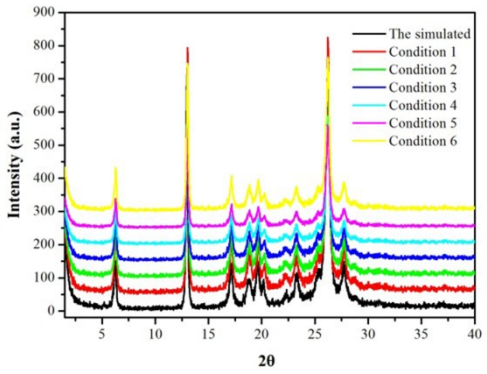
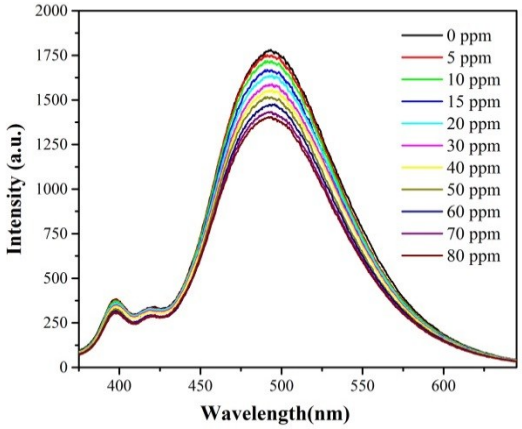


Fig. S5 The PXRD pattern based on the X-ray single crystal diffraction of the compound **2** and the experimental samples of the conditions **1–6**, respectivel.

6. Fluorescence Spectroscopy



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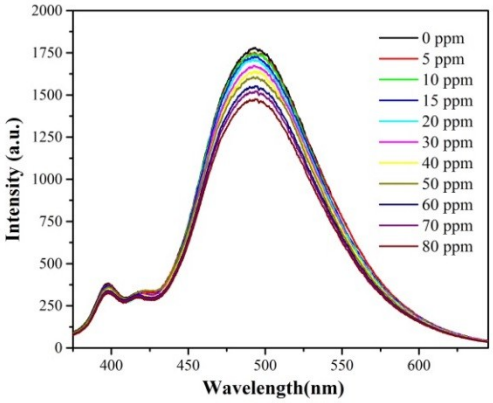

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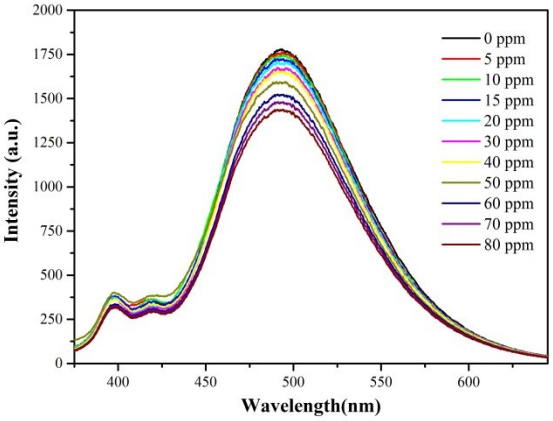

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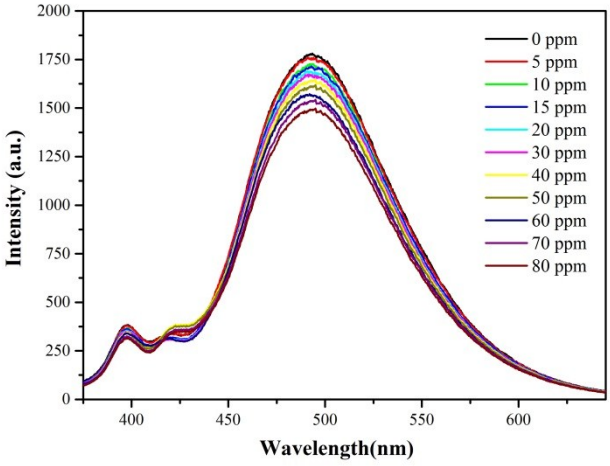
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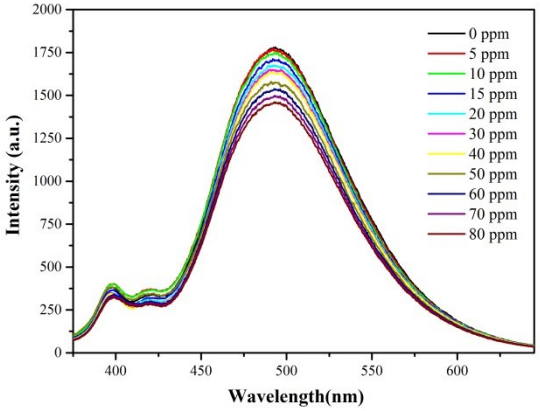
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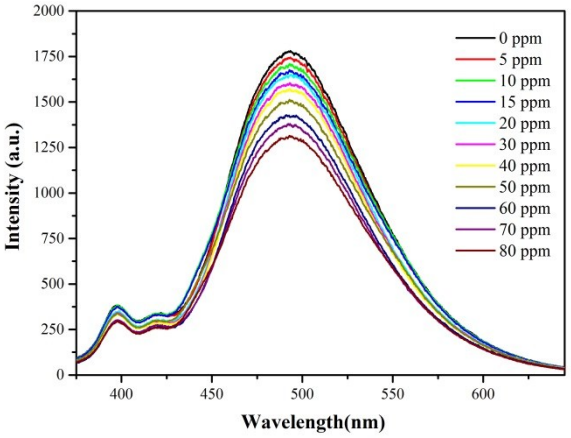
(e)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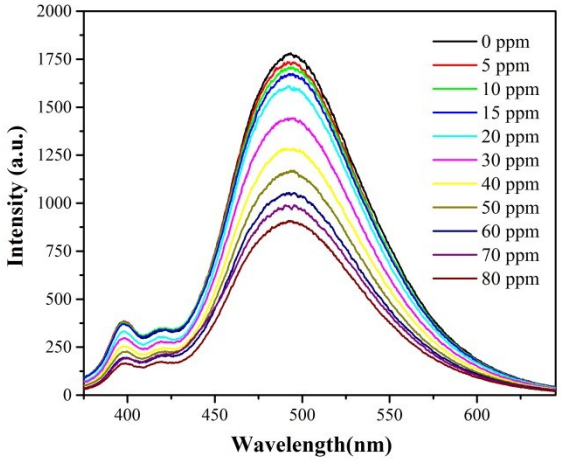
(f)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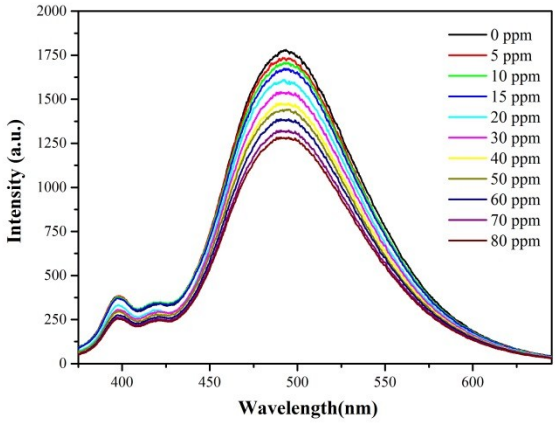
(g)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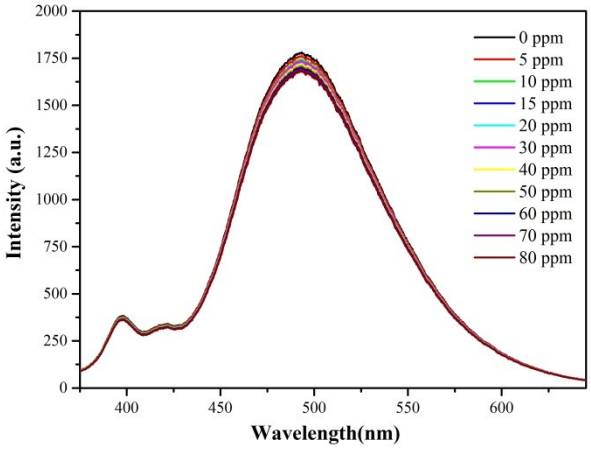
(h)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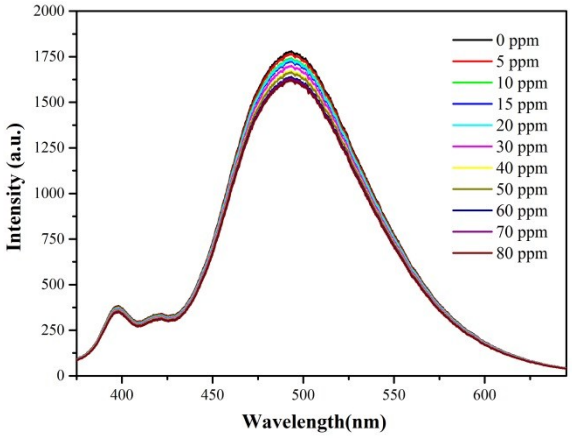
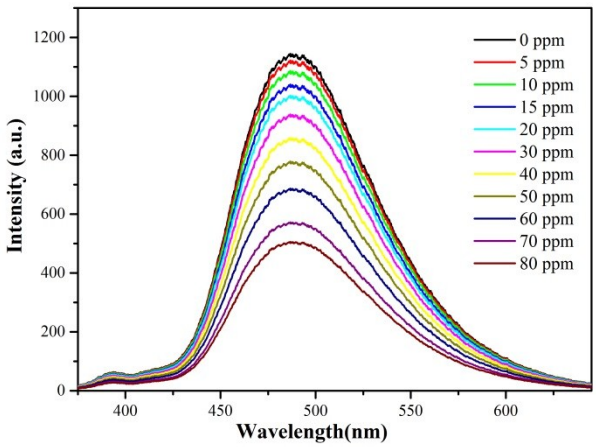
(i)



(j)

Fig. S6 Fluorescence quenching of sensor **2** dispersed in V_{CH_3CN}:V_{H_2O}=1:9 by gradually increasing different quenchers' concentration: (a) 2,4-DNT, (b) 4-Cl-NB, (c) 1,4-DNB, (d) 4-NBA, (e) 1,3-DNB, (f) 1,2-DNB, (g) 2-NP, (h) NB, (i) Phe, (j) m-Thb.



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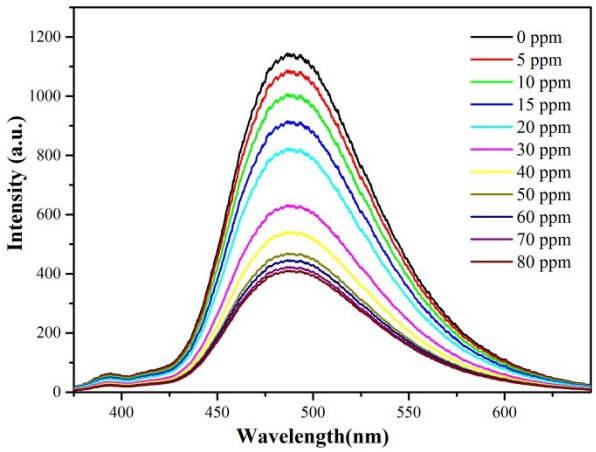
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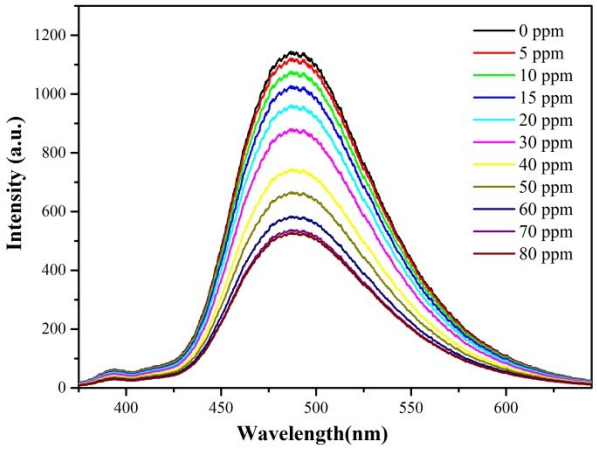
(b)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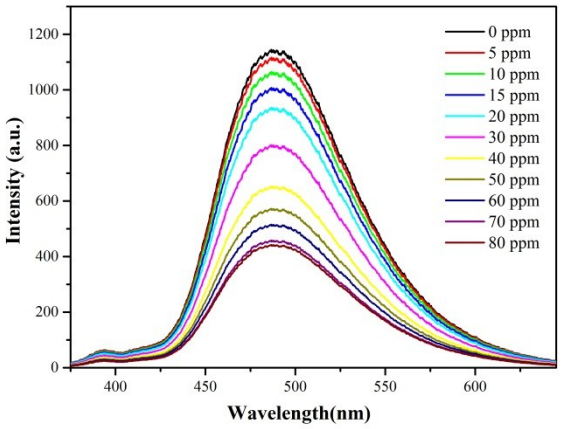
(c)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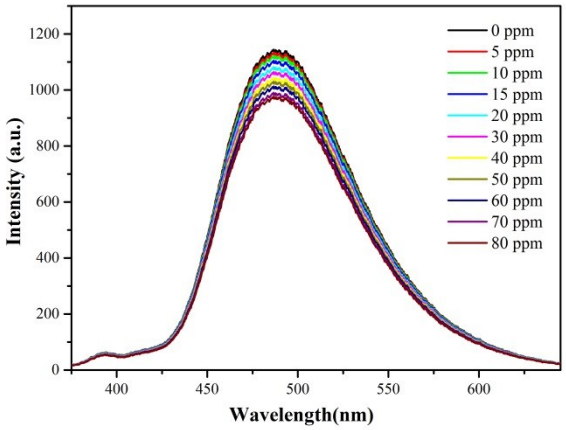
（d）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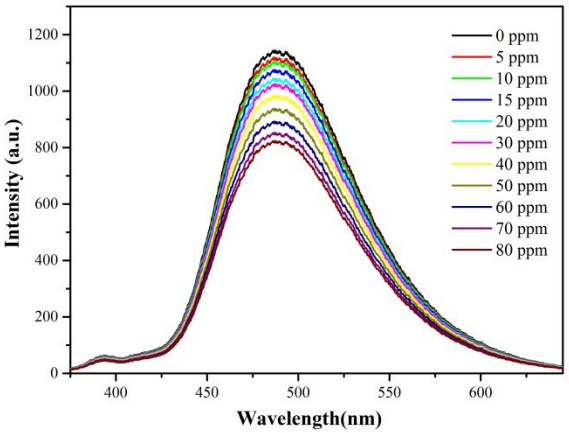
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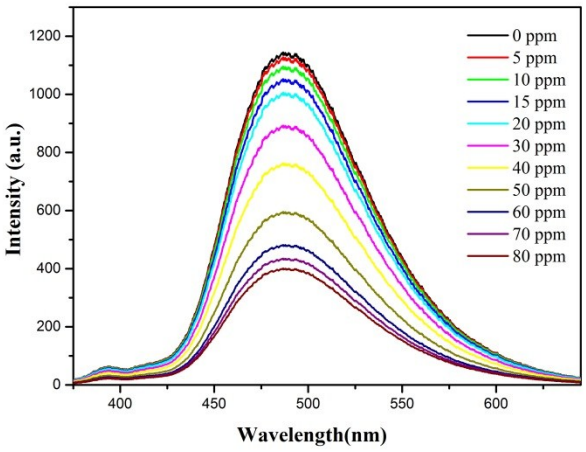
(f)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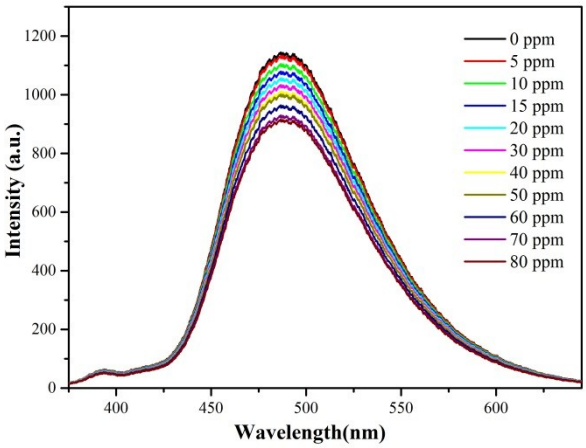

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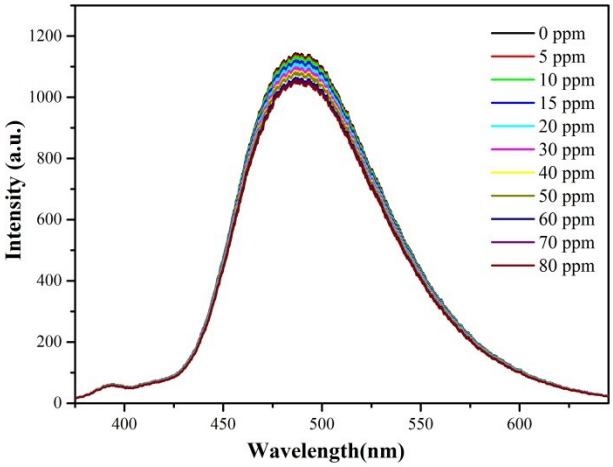

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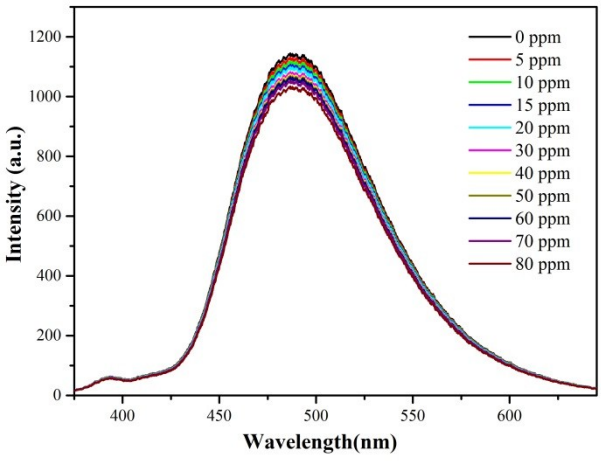

(j)

Fig. S7 Fluorescence quenching of sensor **3** dispersed in V_{DMSO}:V_{H_2O}=1:9 by gradually increasing different

quenchers' concentration: (a) 2,4-DNT, (b) 4-Cl-NB, (c) 1,4-DNB, (d) 4-NBA, (e) 1,3-DNB, (f) 1,2-DNB, (g) 2-NP, (h) NB, (i) Phe, (j) m-Thb.

7. Comparative study of the present system with previously reported systems

Table S3: Comparative study of the present system with previously reported systems.

Serial No.	Material	Method	Medium	LOD
1	Tris-Imidazolium Derivatives	Fluorescence turn off	DMSO	467 and 354 ppb
2	Isobenzotriazolophanes	Fluorescence turn off	Cyclohexane	19 ppm
3	Phosphole oxide	Fluorescence turn off	10 % THF in water	2.03 mM
4	Triphenylamine Derivatives	Fluorescence turn off	Aqueous THF (7:3)	443 ppb
5	Sodium dodecyl sulfate	Fluorescence turn off	Aqueous	1μM
6	Fluorene Derivatives	Fluorescence turn off	CH_3CN	1.39μM
7	Benzo[c]cinnoline Derivatives	Fluorescence turn off	Aqueous CH_3CN (9:1) Aqueous DMSO(9:1)	0.95 μM 1.65 μM

[1 ref. 1; **2** ref. 2; **3** ref. 3; **4** ref. 4; **5** ref. 5; **6** ref. 6], **7**-the present work.

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