Supporting Information

A series of CuX (X = Br, I) modules bearing Ba-MOFs: Structures, fluorescence and sensing properties

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Materials

All reagents and chemicals were purchased from commercial sources and used without further purification. The detailed information for the reagents is listed as follows: Barium nitrate ($Ba(NO_3)_2$, 99%, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); potassium iodide (KI, 99.9%, Adamas Reagent Co., Ltd., Shanghai, China); copper(I) iodide (CuI, 99%, Adamas Reagent Co., Ltd., Shanghai, China); copper(I) bromide (CuBr, 99%, Adamas Reagent Co., Ltd., Shanghai, China); isonicotinic acid ($C_6H_5NO_2$, 99%, Adamas Reagent Co., Ltd., Shanghai, China); 3-fluoroisonicotinic acid ($C_6H_4FNO_2$, 98%, Adamas Reagent Co., Ltd., Shanghai, China); acetonitrile (CH_3CN, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); N,N-dimethylformamide (DMF, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); ethanol (EtOH, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); dimethyl sulfoxide (DMSO, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); ethyl acetate (EA, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); methanol (CH_3OH, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); N,N-dimethylacetamide (DMA, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China); ethylene glycol (EG, AR, Sinopharm Chemical Reagent Co., Ltd., Shanghai, China),

Methionine ($C_5H_{11}NO_2S$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China); reduced glutathione (GSH) (98%, Adamas-life Science, Shanghai, China); L-cysteine monohydrochloride ($C_3H_7NO_2S{\cdot}HCl$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China); (S)-2-amino-4-mercaptobutanoic acid ($C_4H_9NO_2S$, 95%+, Adamas Reagent Co., Ltd., Shanghai, China); phenylalanine ($C_9H_{11}NO_2$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China); glycine ($C_2H_5NO_2$, 99%, Adamas Reagent Co., Ltd., Shanghai, China); L-tryptophan ($C_{11}H_{12}N_2O_2$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China); L-aspartic acid ($C_4H_7NO_4$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China); tyrosine ($C_9H_{11}NO_3$, BR, Tianjin Guangfu Science and Technology Development Co., Ltd., Tianjin, China).

Deionized water was prepared in our laboratory by purification using a Water Purifier (Watepur®) ultrapure water system. All reagents for synthesis were commercially available and used as received without further purification.

Table S1. Crystal data and structure refinement details for title compounds.

Compounds	**1**	**2**	**3**
Empirical formula	$C_{24}H_{14}Ba_2Br_2Cu_2F_4N_4O_9$	$C_{30}H_{33}Ba_2Br_3Cu_4N_5O_{16.5}$	$C_{69}H_{68}Ba_2Cu_7I_6K_5N_{13}O_{26.5}$
CCDC number	2504604	2504605	2504606
Formula weight	1139.970	1496.18	3179.72
Temperature/K	280K	100K	100K
Wavelength/Å	0.71073	0.71073	0.71073
Crystal system	orthorhombic	triclinic	triclinic
Space group	*Pbcm*	*P*-1	*P*-1
a/Å	7.0307(3)	9.2951(2)	10.6665(2)
b/Å	12.5506(6)	11.6513(2)	14.1811(3)
c/Å	32.7980(14)	20.1943(4)	18.5074(3)
α/°	90	74.916(2)	105.729(2)
β/°	90	81.305(2)	102.660(2)
γ/°	90	86.706(2)	100.660(2)
Volume/$Å^3$	2894.1(2)	2087.04(7)	2535.42(9)
Z	4	2	1
ρ_{calc} g/cm^3	2.616	2.381	2.083
Absorption coefficient/mm^{-1}	6.983	6.806	4.305
F(000)	2136	1426	1513
Crystal size/mm^3	0.30×0.20×0.10	0.30×0.10×0.05	0.30×0.20×0.20
Reflections collected/ unique	14713/3769	31367/10718	39536/15510
	[R_{int} = 0.0368]	[R_{int} = 0.0339]	[R_{int} = 0.0335]
Data/restraints/parameters	3769/1/229	10718/18/586	15510/282/711
Goodness-of-fit on F_2	1.07	1.034	1.060
Final *R* indexes [$I >= 2\sigma(I)$]	R_1[a] = 0.0429,	R_1[a] = 0.0295,	R_1[a] = 0.0381,
	wR_2 [b]= 0.0899	wR_2[b] =0.0658	wR_2 [b]= 0.0906
Final *R* indexes [all data]	R_1 [a]= 0.0664,	R_1[a] = 0.0411,	R_1[a] = 0.0552,
	wR_2 [b]= 0.1011	wR_2[b] = 0.0691	wR_2 [b]= 0.0972

[a] $R_1 = \Sigma \| F_o | - | F_n \| / \Sigma | F_o |$, [b] $wR_2 = [\Sigma w(| F_o |^2 - | F_n |^2)^2 / \Sigma w(|F_o|^2)^2]^{1/2}$

Table S2. Selected bond lengths (Å) for compound **1**.

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Ba(1)-O(1W)	3.007(6)	Br(1)-Cu(1B)$^{\#6}$	2.842(13)
Ba(1)-O(1W)	2.794(4)	Br(1)-Cu(2)$^{\#6}$	2.6152(18)
Ba(1)-O(1)$^{\#1}$	2.730(4)	Br(2)-Cu(1)	2.6588(19)
Ba(1)-O(2)$^{\#2}$	2.749(4)	Br(2)-Cu(1B)	2.588(10)
Ba(1)-O(2)	3.030(5)	Br(2)-Cu(2)	2.5918(19)
Ba(1)-O(3)$^{\#3}$	3.187(5)	Cu(1)-N(1)$^{\#7}$	1.997(5)
Ba(1)-O(3)$^{\#4}$	2.813(5)	Cu(1)-N(1)	1.997(5)
Ba(1)-O(4)$^{\#3}$	2.825(4)	Cu(1B)-N(1)$^{\#7}$	1.953(6)
Ba(1)-O(4)$^{\#5}$	2.755(4)	Cu(2)-N(2)	2.035(5)
Br(1)-Cu(1)	2.568(2)	Cu(2)-N(2)$^{\#7}$	2.035(5)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$1-*x*,1-*y*,1-*z*; $^{\#2}$-*x*,1-*y*,1-*z*; $^{\#3}$-1+*x*,+*y*,1/2-*z*; $^{\#4}$1-*x*,1-*y*,1/2+*z*; $^{\#5}$-1+*x*,1/2-*y*,1/2+*z*; $^{\#6}$1-*x*,1/2+*y*,1/2-*z*; $^{\#7}$+*x*,+*y*,1/2-*z*

Table S3. Hydrogen bonding data for compound **1**.

D−H···A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å
O(1W)-H(1)···O(3)$^{\#1}$	0.821(10)	2.42(7)	3.050(8)
C(1)-H(1A)···Br(2)	0.93	2.83	3.464(6)
C(5)-H(5A)···Br(2)$^{\#2}$	0.93	2.68	3.609(6)
C(7)-H(7A)···Br(1)$^{\#3}$	0.93	2.79	3.699(7)
C(11)-H(11A)···Br(1)$^{\#4}$	0.93	2.81	3.497(6)

Symmetry transformations used to generate equivalent atoms:$^{\#1}$+*x*,1/2-*y*,1/2+*z*; $^{\#2}$-1+*x*,+*y*,+*z*; $^{\#3}$2-*x*,-1/2+*y*,1/2-*z*; $^{\#4}$1-*x*,-1/2+*y*,1/2-*z*

Table S4. Selected bond lengths (Å) for compound **2**.

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Ba(1)-O(1)	4.5161(3)	Ba(2)-O(6W)	2.953(3)
Ba(1)-O(2)	3.212(3)	Ba(2)-O(7W)	2.765(3)
Ba(1)-O(4)$^{\#1}$	2.783(3)	Br(1)-Cu(1)	2.6179(6)
Ba(1)-O(10)$^{\#2}$	2.775(3)	Br(1)-Cu(2)	2.5964(6)
Ba(1)-O(1W)$^{\#3}$	2.683(3)	Br(1)-Cu(3)$^{\#8}$	2.8439(7)
Ba(1)-O(1W)	2.854(6)	Br(1)-Cu(3)	2.5340(6)
Ba(1)-O(2W)	2.974(6)	Br(2)-Cu(2)	2.5437(6)
Ba(1)-O(3W)	2.760(3)	Br(2)-Cu(3)	2.3736(6)
Ba(1)-O(4W)	2.867(3)	Br(2)-Cu(4)	2.4861(6)
Ba(1)-O(5W)	2.871(3)	Br(3)-Cu(2)	2.4646(6)
Ba(2)-O(1)	4.4990(4)	Br(3)-Cu(4)	2.4931(6)
Ba(2)-O(5)$^{\#5}$	2.678(3)	Br(3)-Cu(4)$^{\#2}$	2.5793(6)
Ba(2)-O(5)$^{\#6}$	2.723(2)	Cu(1)-N(1)	1.944(3)
Ba(2)-O(6)$^{\#6}$	2.961(3)	Cu(1)-N(2)	1.930(3)

Ba(2)-O(7)#7	2.837(2)	Cu(2)-N(3)	2.001(3)
Ba(2)-O(3W)	2.729(3)	Cu(3)-N(4)	1.968(3)
Ba(2)-O(4W)	2.870(3)	Cu(4)-N(5)	2.007(3)

Symmetry transformations used to generate equivalent atoms: #1 1-*x*,-*y*,1-*z*; #2 -*x*,-*y*,1-*z*; #3 1-*x*,-*y*,-*z*; #4 2-*x*,1-*y*,-*z*; #5 1+*x*,+*y*,+*z*; #6 1-*x*,1-*y*,-*z*; #7 1-*x*,1-*y*,1-*z*; #8 -*x*,1-*y*,1-*z*

Table S5. Hydrogen bonding data for compound **2**.

D−H···A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O(1W)-H(1A)···O(4)#1	0.821(10)	2.16(7)	2.843(6)	140(9)
O(1W)-H(1A)···O(6W)#2	0.821(10)	2.62(7)	3.088(7)	118(7)
O(1W)-H(1B)···O(10)#3	0.820(10)	2.40(9)	2.907(6)	120(9)
O(1W)-H(1B)···O(2W)#4	0.820(10)	2.63(8)	3.146(7)	122(8)
O(2W)-H(2A)···O(3)#1	0.828(10)	1.960(18)	2.764(4)	163(4)
O(2W)-H(2B)···O(8)#5	0.827(10)	1.975(13)	2.788(4)	167(4)
O(3W)-H(3A)···O(7W)#2	0.821(10)	2.092(19)	2.880(4)	161(5)
O(3W)-H(3B)···O(6)	0.819(10)	2.18(3)	2.873(4)	142(4)
O(4W)-H(4A)···O(8)#5	0.824(10)	1.925(11)	2.747(4)	175(4)
O(4W)-H(4B)···O(5)#6	0.824(10)	2.44(5)	2.912(4)	117(4)
O(4W)-H(4B)···O(9)#7	0.824(10)	2.44(3)	3.146(4)	145(4)
O(5W)-H(5A)···O(8)#7	0.83	2.19	2.885(5)	141.8
O(5W)-H(5B)···O(9)#7	0.82	2.11	2.836(4)	146.7
O(6W)-H(6A)···O(9)#8	0.819(10)	1.924(14)	2.735(4)	170(6)
O(6W)-H(6B)···O(4)#9	0.820(10)	2.51(3)	3.215(4)	144(5)
O(6W)-H(6B)···O(7)#9	0.820(10)	2.53(4)	3.010(4)	118(4)
O(7W)-H(7A)···O(3)#9	0.822(10)	1.925(14)	2.737(4)	169(5)
O(7W)-H(7B)···O(6)	0.821(10)	1.93(2)	2.704(4)	158(5)
C(7)-H(7)···Br(1)#9	0.95	3	3.864(4)	151.9
C(10)-H(10)···O(2)#7	0.95	2.46	3.133(5)	128.2
C(11)-H(11A)···Br(3)	0.95	3.05	3.818(4)	139.5
C(13)-H(13A)···Br(2)	0.95	3.12	3.751(4)	125.7
C(14)-H(14A)···O(7)#10	0.95	2.63	3.273(5)	125.1
C(19)-H(19A)···Br(1)	0.95	3.07	3.683(4)	123.5
C(25)-H(25A)···Br(3)	0.95	3.11	3.756(4)	126.5

Symmetry transformations used to generate equivalent atoms: #1 +*x*,+*y*,-1+*z*; #2 1-*x*,1-*y*,-*z*; #3 -*x*,-*y*,1-*z*; #4 1-*x*,-*y*,-*z*; #5 1+*x*,+*y*,-1+*z*; #6 1+*x*,+*y*,+*z*; #7 1-*x*,-*y*,1-*z*; #8 1+*x*,1+*y*,-1+*z*; #9 1-*x*,1-*y*,1-*z*; #10 -*x*,1-*y*,1-*z*

Table S6. Selected bond lengths (Å) for compound **3**.

Atom-Atom	**Length/Å**	**Atom-Atom**	**Length/Å**
Ba(1)-O(2)	2.711(4)	Cu(4)-N(5)$^{\#6}$	1.953(3)
Ba(1)-O(3)$^{\#1}$	2.847(3)	Cu(4)-N(5)	1.953(3)
Ba(1)-O(4)$^{\#1}$	2.760(3)	K(1)-O(1)	2.652(5)
Ba(1)-O(5)$^{\#2}$	2.798(3)	K(1)-O(3)$^{\#7}$	2.743(5)
Ba(1)-O(5)$^{\#3}$	2.860(4)	K(1)-O(5)	2.944(4)
Ba(1)-O(6)$^{\#3}$	2.915(3)	K(1)-O(6)	3.374(5)
Ba(1)-O(7)$^{\#4}$	2.927(4)	K(1)-O(8)$^{\#8}$	2.607(5)
Ba(1)-O(9)	2.652(4)	K(1)-O(9)$^{\#3}$	3.109(5)
Ba(1)-O(8)$^{\#4}$	2.867(4)	K(1)-O(10)$^{\#3}$	2.883(5)
I(1)-Cu(1)	2.6563(6)	K(1)-O(12)	2.739(13)
I(1)-Cu(2)	2.6491(6)	K(2)-O(1)	2.895(3)
I(1)-Cu(3)	2.6572(6)	K(2)-O(2)	2.926(3)
I(2)-Cu(1)	2.7000(6)	K(2)-O(6)$^{\#3}$	3.018(4)
I(2)-Cu(3)	2.6402(6)	K(2)-O(7)$^{\#4}$	2.668(4)
I(2)-Cu(4)	3.2390(3)	K(2)-O(10)$^{\#3}$	2.682(3)
I(3)-Cu(2)$^{\#5}$	2.6533(5)	K(2)-O(11)	2.811(8)
I(3)-Cu(2)	2.5996(5)	K(2)-O(12)	2.815(10)
I(3)-Cu(3)	2.7018(6)	K(3)-O(1)	2.720(3)
I(3)-Cu(4)	3.1853(2)	K(3)-O(1)$^{\#3}$	2.720(3)
Cu(1)-N(1)	2.011(3)	K(3)-O(6)	2.619(3)
Cu(1)-N(2)	2.009(3)	K(3)-O(6)$^{\#3}$	2.619(3)
Cu(2)-N(3)	2.044(3)	K(3)-O(10)$^{\#3}$	2.776(3)
Cu(3)-N(4)	2.061(3)	K(3)-O(10)	2.776(3)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$1-*x*,2-*y*,1-*z*; $^{\#2}$-1+*x*,+*y*,+*z*; $^{\#3}$1-*x*,1-*y*,-*z*; $^{\#4}$-1+*x*,+*y*,-1+*z*; $^{\#5}$2-*x*, 1-*y*,1-*z*; $^{\#6}$1-*x*,1-*y*,1-*z*; $^{\#7}$2-*x*,2-*y*,1-*z*; $^{\#8}$+*x*,+*y*,-1+*z*

Table S7. Hydrogen bonding data for compound **3**.

D−H···A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
C(3)-H(3A)···O(4)$^{\#1}$	0.95	2.43	3.364(5)	168.9
C(5)-H(5A)···I(1)	0.95	3.31	3.935(4)	125.4
C(10)-H(10A)···I(1)	0.95	3.23	3.835(4)	123.4
C(17)-H(17A)···I(3)$^{\#2}$	0.95	3.25	3.846(4)	122.9
C(21)-H(21A)···O(11)$^{\#3}$	0.95	2.52	3.408(11)	156.0
C(22)-H(22A)···I(1)	0.95	3.27	3.873(4)	122.9
C(23)-H(23A)···I(2)	0.95	3.23	3.852(5)	125.1
C(28)-H(28A)···I(2)	0.95	3.27	3.748(4)	113.3
C(28)-H(28A)···I(3)$^{\#4}$	0.95	3.29	3.744(4)	111.4

C(29)-H(29A)···I(2)#4	0.95	3.25	3.714(4)	112.4
C(29)-H(29A)···I(3)	0.95	3.15	3.621(4)	112.7
C(30)-H(30A)···O(11)#5	0.95	2.49	3.400(9)	160.8
C(31B)-H(31B)···I(2)#6	0.95	3.15	3.937(11)	141.4
C(32B)-H(32F)···I(2)#6	0.98	3.16	4.031(15)	148.6
C(35)-H(35A)···O(7)#7	0.98	2.43	3.050(19)	120.6

Symmetry transformations used to generate equivalent atoms: #1 1-*x*,2-*y*,1-*z*; #2 2-*x*,1-*y*,1-*z*; #3 1+*x*,+*y*,1+*z*; #4 1-*x*,1-*y*,1-*z*; #5 1-*x*,1-*y*,-*z*; #6 +*x*,+*y*,-1+*z*; #7 2-*x*,2-*y*,1-*z*

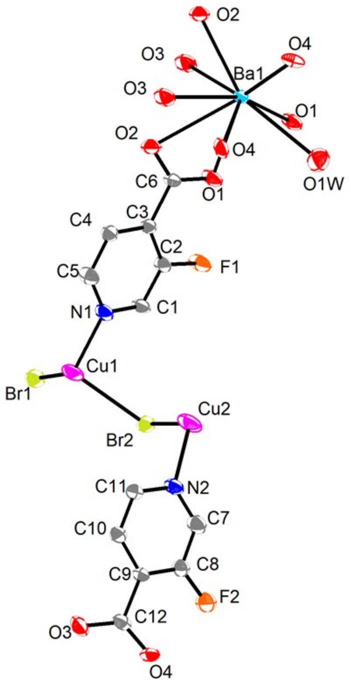

Figure S1. *Ortep* drawing of the asymmetric unit of compound **1** (drawn at 50% probability level); hydrogen atoms are omitted for clarity.

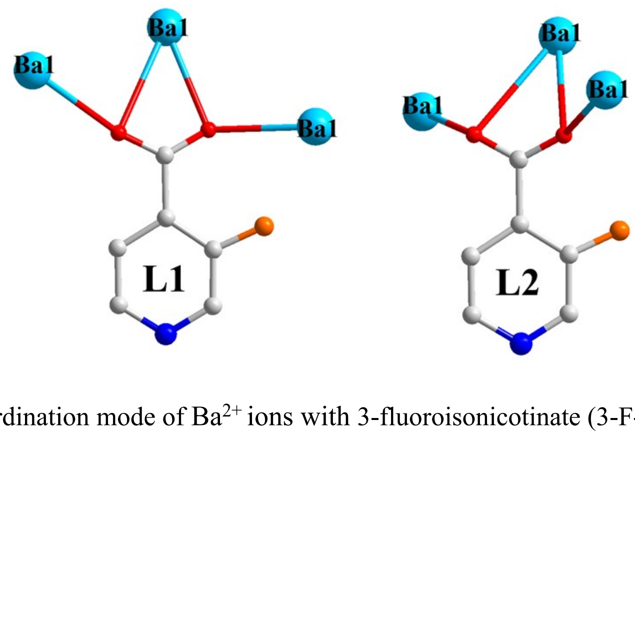

Figure S2. The coordination mode of Ba^{2+} ions with 3-fluoroisonicotinate (3-F- INA^-) in compound **1**.

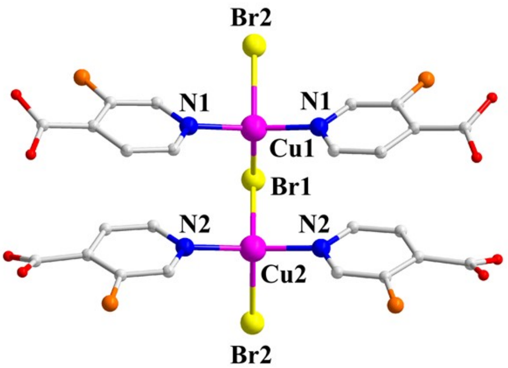

Figure S3. The coordination mode of the $\{Cu_2Br_2\}_n$ unit with the 3-F- INA^- ligand in compound **1**.

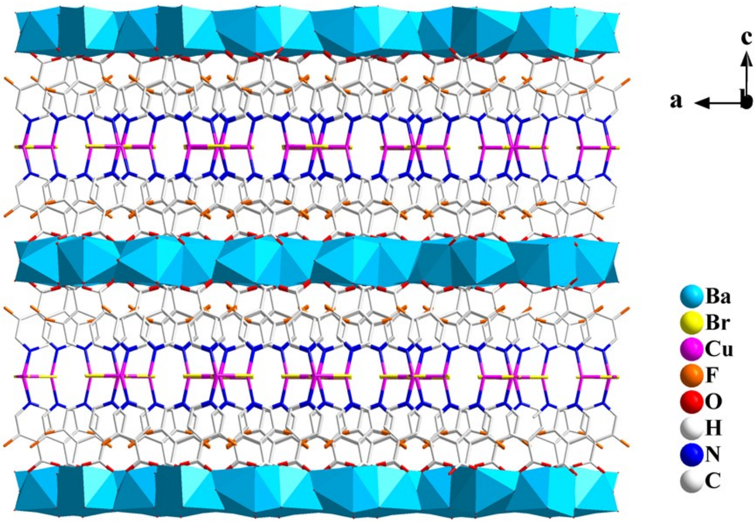

Figure S4. The 3D framework of compound **1** viewed along the *b*-axis.

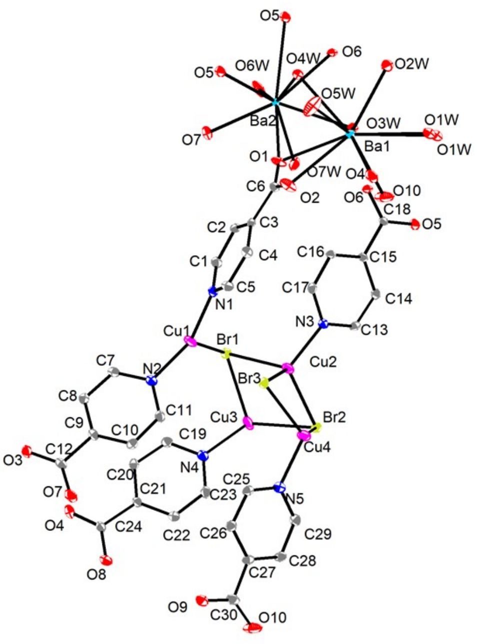

Figure S5. *Ortep* drawing of the asymmetric unit of compound **2** (drawn at 50% probability level); hydrogen atoms are omitted for clarity.

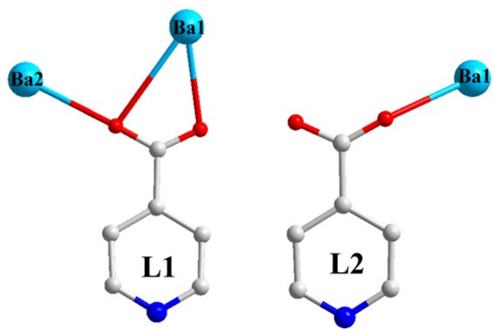

Figure S6. The coordination mode of Ba^{2+} ions with INA^{-} ligand in compound **2.**

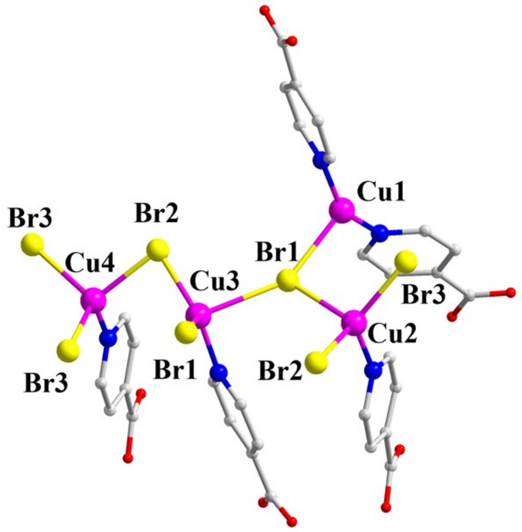

Figure S7. The coordination mode of the $\{Cu_4Br_3\}_n^{n+}$ unit with the INA^{-} ligand in compound **2**.

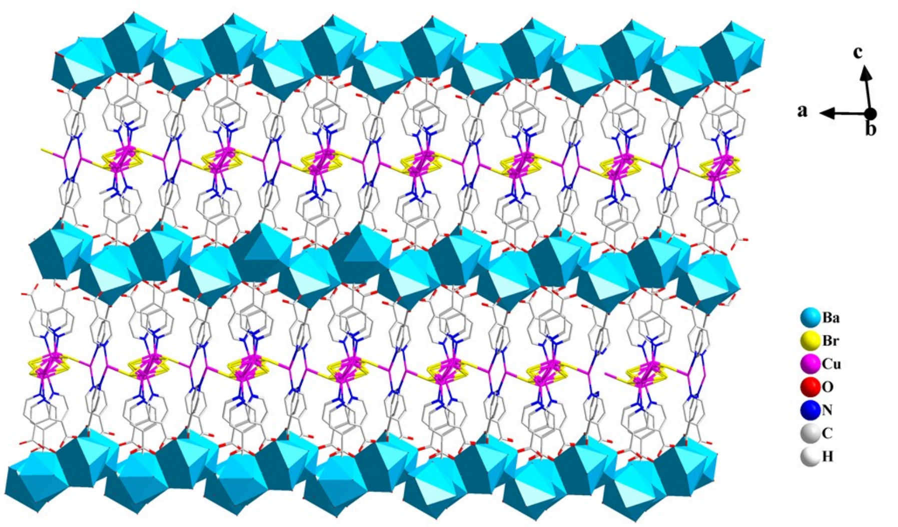

Figure S8. The 3D framework of compound **2** viewed along the *b*-axis.

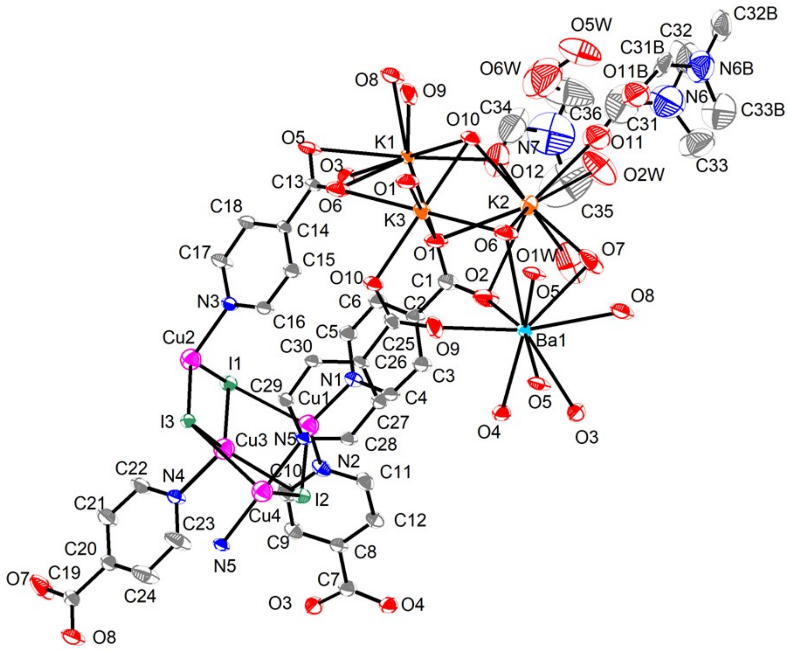

Figure S9. *Ortep* drawing of the asymmetric unit of compound **3** (drawn at 50% probability level); hydrogen atoms are omitted for clarity.

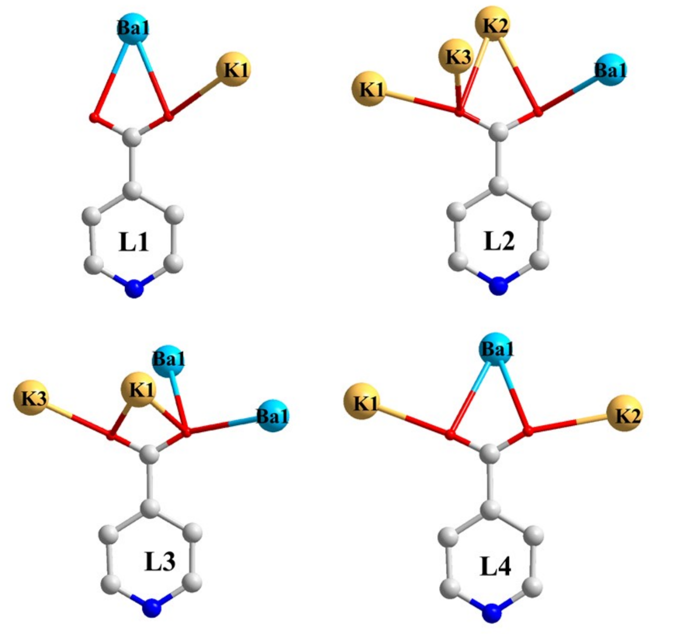

Figure S10. The coordination modes of Ba^{2+} and K^{+} ions with INA^{-} ligands in compound **3**.

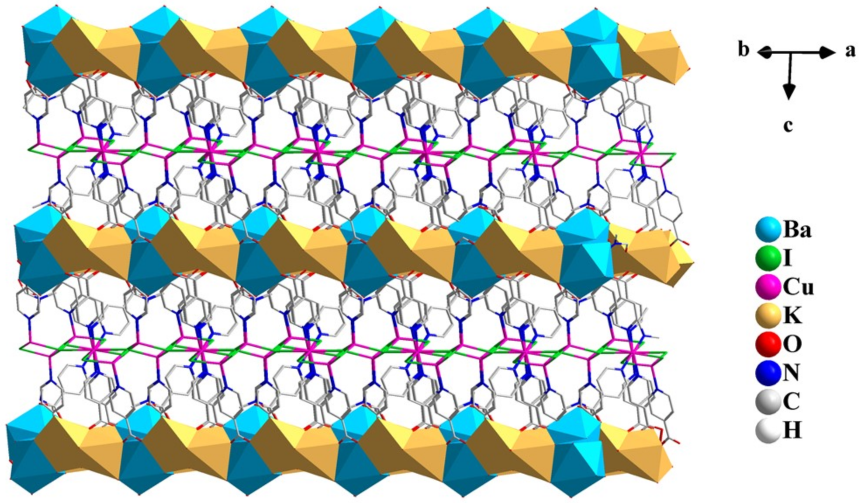

Figure S11. The 3D framework of compound **3** viewed along the [101] direction.

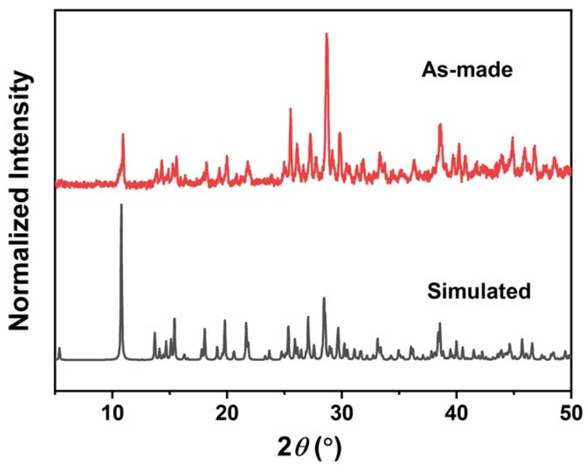

Figure S12. The PXRD pattern for the as-made compound **1**. The simulated pattern is included for comparison.

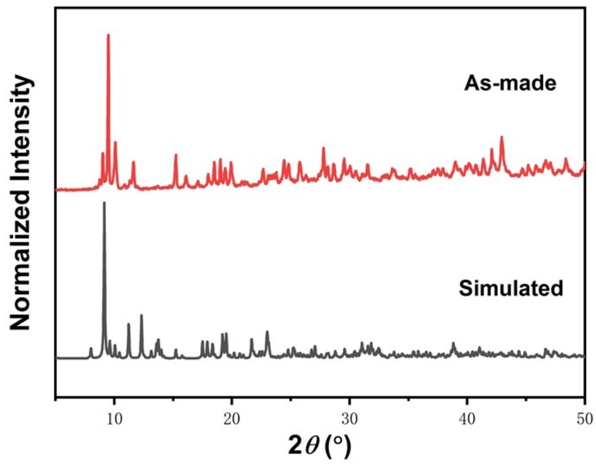

Figure S13. The PXRD pattern for the as-made compound **2**. The simulated pattern is included for comparison.

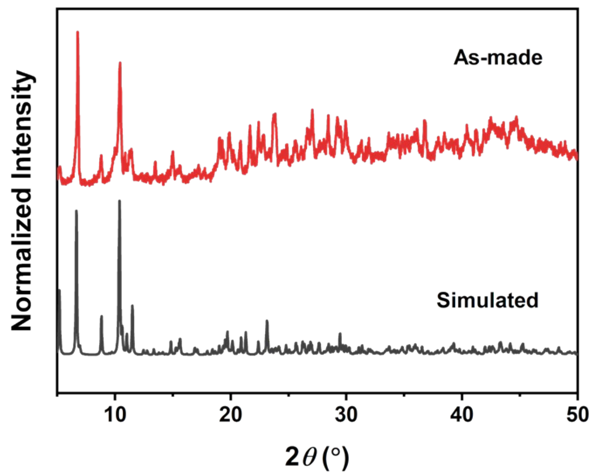

Figure S14. The PXRD pattern for the as-made compound **3**. The simulated pattern is included for comparison.

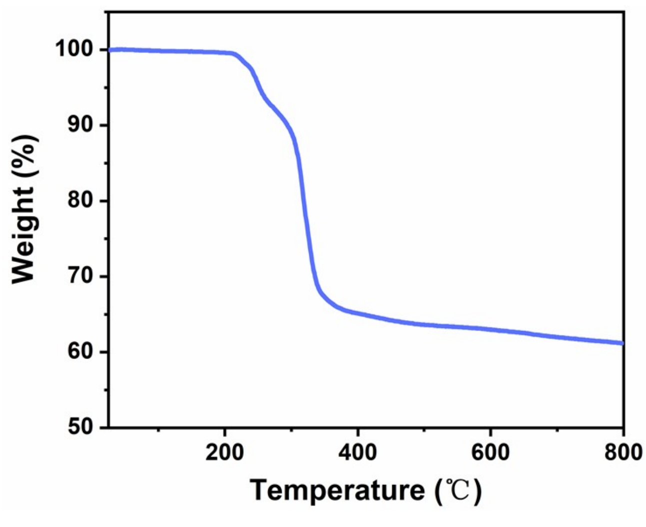

Figure S15. The TG curve for the as-made compound **1**.

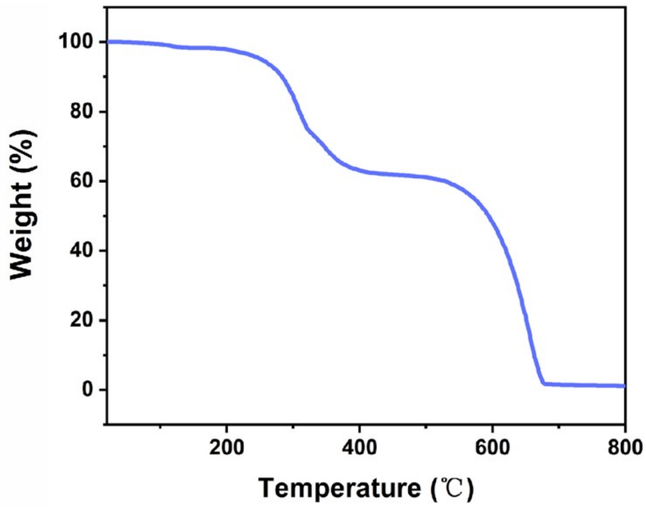

Figure S16. The TG curve for the as-made compound **2.**

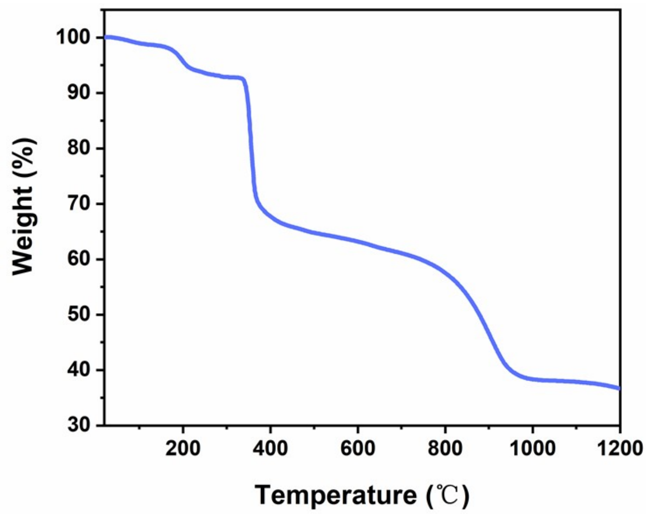

Figure S17. The TG curve for the as-made compound **3.**

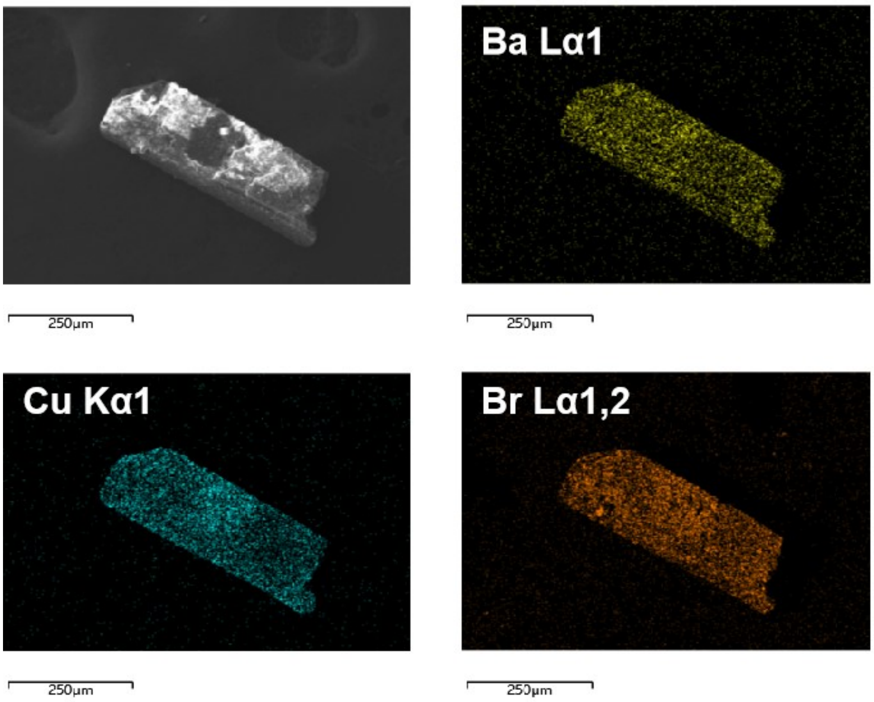

Figure S18. SEM images and corresponding elemental mapping images of Ba, Cu, and Br in compound **2**.

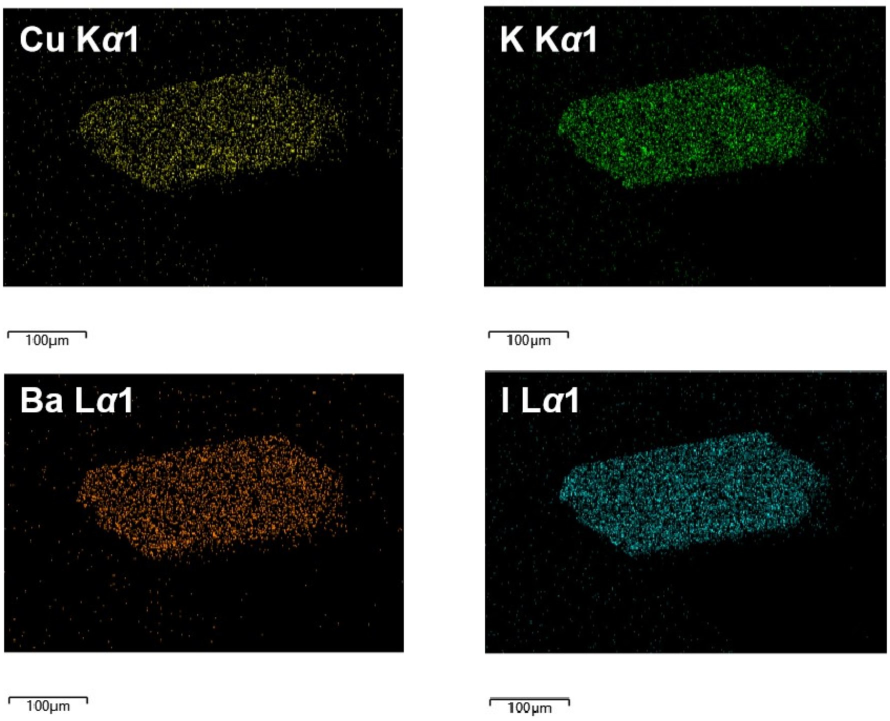

Figure S19. SEM images and corresponding elemental mapping images of Ba, K, Cu, and I in compound **3**.

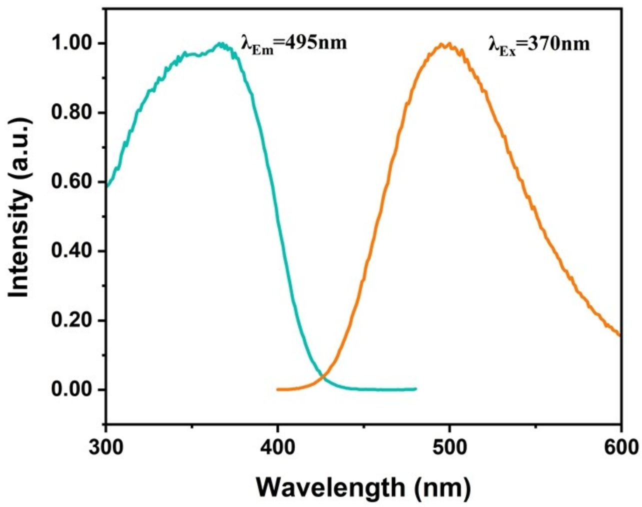

Figure S20. The excitation and emission spectra for the as-made compound **2**.

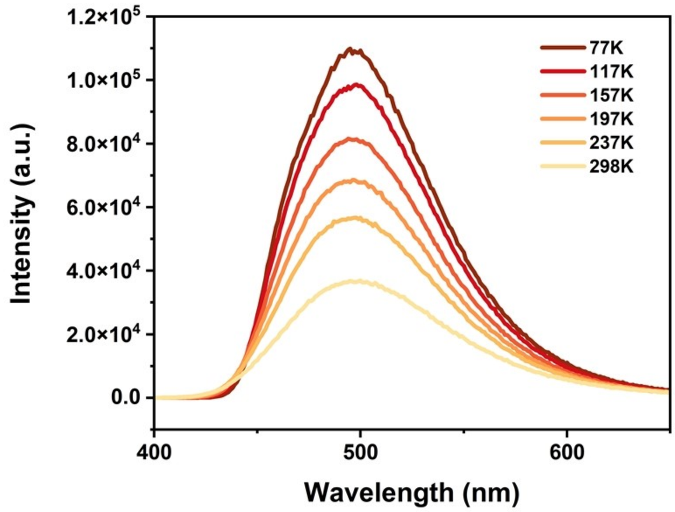

Figure S21. The excitation and emission spectra for the compound **2**.

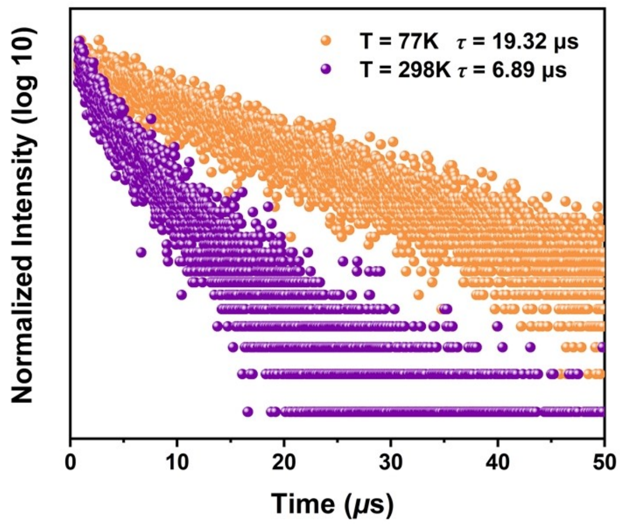

Figure S22. Fluorescence lifetime plot of compound **2**.

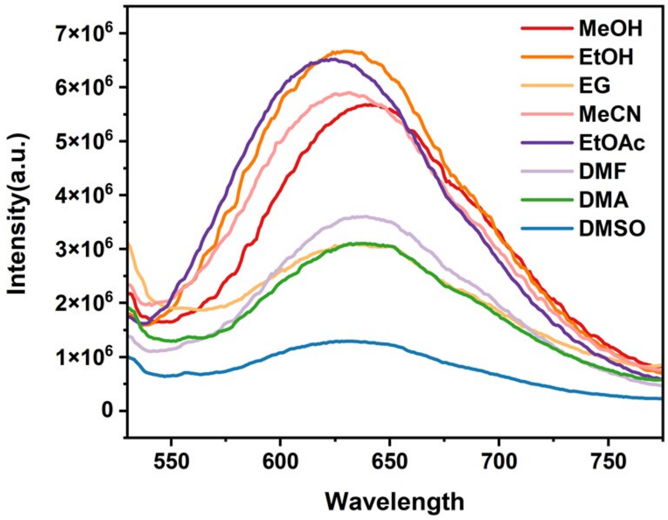

Figure S23. The fluorescence spectra of compound **3** dispersed in different solvents.

Table S8. Comparison of the Cys and Fe^{3+} sensing performances for compound **3** and other reported materials.

Reference	Material	Analytes	R^2	*K*sv / (L·mol⁻¹)
This work	$Ba_2K_5(DMF)_4[Cu_7I_6(INA)_{10}](H_2O)_3$	Fe^{3+}	0.9790	5.92×10^4
1	$[Eu(BCB)(DMF)]\cdot(DMF)_{1.5}(H_2O)_2$	Fe^{3+}	0.9970	2.35×10^4
2	Tb-MOF	Fe^{3+}	0.9970	1.6257×10^5
3	Acridine derivative L1	Fe^{3+}	0.9924	1.03×10^4
4	JLJU-2	Fe^{3+}	0.9462	1.32×10^3
	JLJU-3	Fe^{3+}	0.9992	1.71×10^3
This work	$Ba_2K_5(DMF)_4[Cu_7I_6(INA)_{10}](H_2O)_3$	Cys	0.9866	2.73×10^4
5	Sr-K-CuI-INA	Cys	0.9928	8.0×10^3
6	$[(Cu_2I_2)_2Ce_2(INA)_6(DMF)_3]\cdot DMF$	Cys	0.9883	1.96×10^4
7	LMOF $\{[(Cu_2I_2)L_2]\cdot 2DMSO\}_n$	Cys	0.9914	6.128×10^2

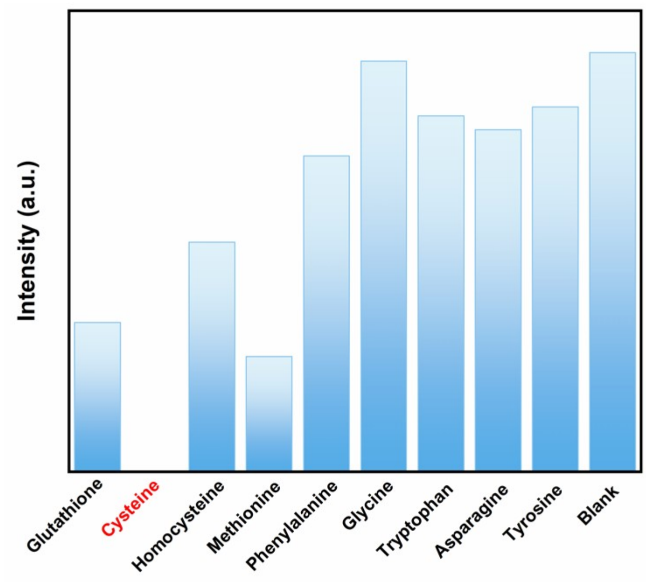

Figure S24. Comparison of fluorescence responses of compound **3** towards different amino acids.

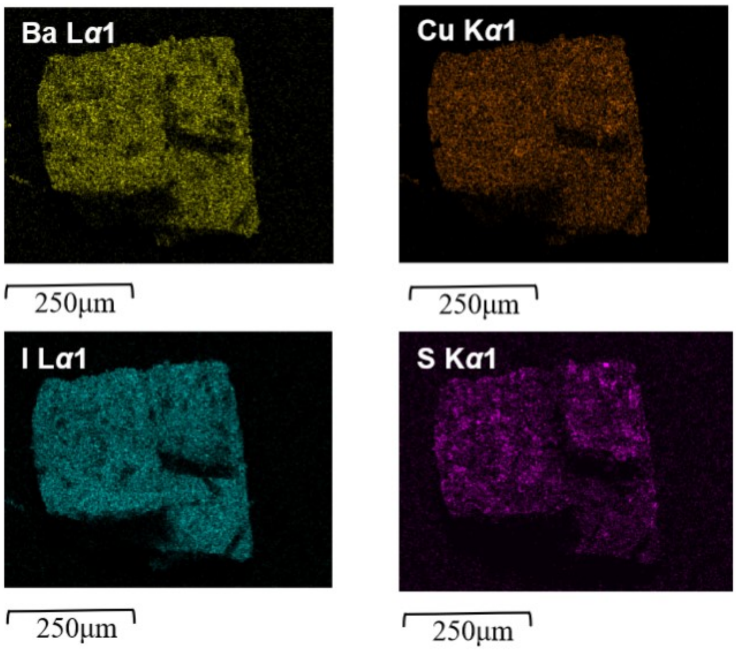

Figure S25. Elemental mapping images of barium (Ba), copper (Cu), iodine (I), and sulfur (S) for compound **3** after Cys sensing.

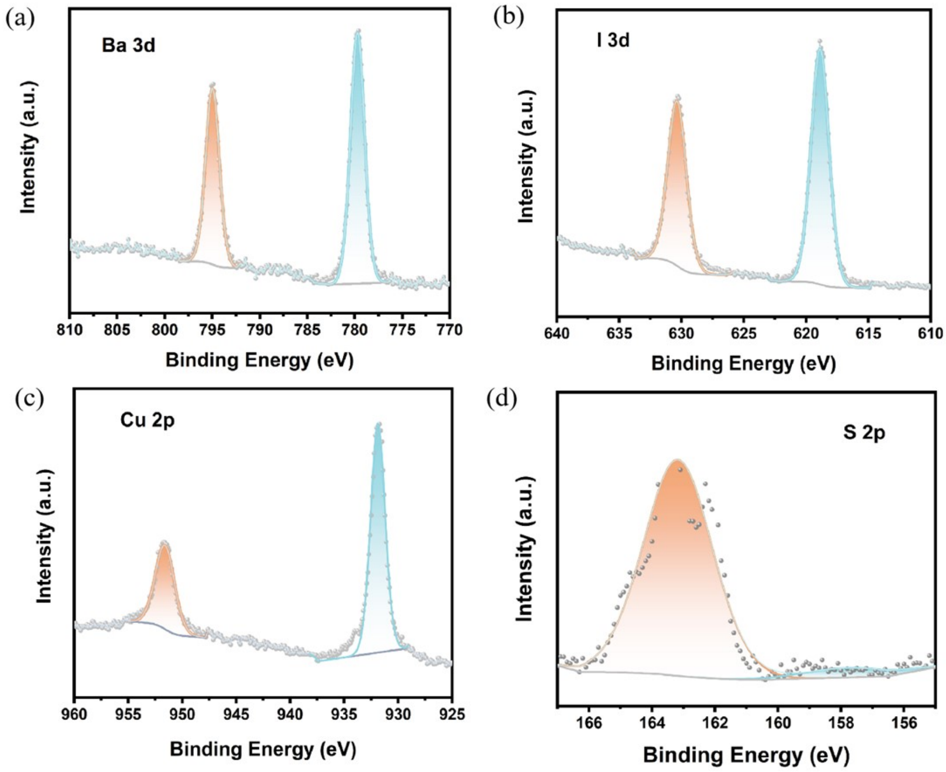

Figure S26. The XPS spectra of Ba 3*d*, I 3*d*, Cu 2*p*, and S 2*p* for the sample of **3** immersed in Cys.

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