A luminescent terbium coordination polymer as a multifunctional water-stable sensor for detection of Pb^{2+} ions, PO_4^{3-} ions, $Cr_2O_7^{2-}$ ions, and some amino acids

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Table S1. The crystallographic data for complex **1**

Complex 1	
Formula	$C_{19}H_{11}NO_8Tb$
Formula Weight	540.21
T/K	293(2)
Crystal System	Monoclinic
Space Group	*C*2/c
a (Å)	28.153(5)
b (Å)	7.2450(5)
c (Å)	21.869(3)
α (°)	90
b (°)	120.140(10)
γ (°)	90
V (A^3)	3857.5(9)
Z	8
D calc.(g cm^{-3})	1.860
μ (mm^{-1})	18.462
F (000)	2088
Rint	0.0312
GOF	1.081
R_1^a	0.0530
ωR_2^b [I > 2*s* (I)]	0.1464
R_1 (all data)	0.0649
ωR_2 (all data)	0.1707
Δr_{max} and $_{min}$ (e $Å^{-3}$)	2.305, -2.026

Table S2. Selected bond lengths [Å] and angles [°] for **1**

Complex 1			
Tb(1)-O(3)	2.356(5)	Tb(1)-O(4)#1	2.458(6)
Tb(1)-O(8)	2.360(6)	Tb(1)-O(2)#2	2.492(5)
Tb(1)-O(2)	2.362(5)	Tb(1)-O(1)#2	2.522(6)
Tb(1)-O(6)	2.376(6)	Tb(1)-O(3)#1	2.553(5)
Tb(1)-O(7)#1	2.405(5)		
O(3)-Tb(1)-O(8)	130.7(2)	O(3)-Tb(1)-O(2)	72.84(18)
O(8)-Tb(1)-O(2)	79.6(2)	O(3)-Tb(1)-O(6)	72.71(19)
O(8)-Tb(1)-O(6)	70.9(2)	O(2)-Tb(1)-O(6)	96.84(19)
O(3)-Tb(1)-O(7)#1	68.84(19)	O(8)-Tb(1)-O(7)#1	142.45(19)
O(2)-Tb(1)-O(7)#1	77.55(18)	O(6)-Tb(1)-O(7)#1	141.09(19)
O(3)-Tb(1)-O(4)#1	139.3(2)	O(8)-Tb(1)-O(4)#1	89.9(2)
O(2)-Tb(1)-O(4)#1	118.92(18)	O(6)-Tb(1)-O(4)#1	135.9(2)
O(7)#1-Tb(1)-O(4)#1	75.9(2)	O(3)-Tb(1)-O(2)#2	71.13(17)
O(8)-Tb(1)-O(2)#2	138.3(2)	O(2)-Tb(1)-O(2)#2	140.13(9)
O(6)-Tb(1)-O(2)#2	88.34(18)	O(7)#1-Tb(1)-O(2)#2	80.34(18)
O(3)-Tb(1)-O(1)#2	111.8(2)	O(8)-Tb(1)-O(1)#2	86.4(2)
O(2)-Tb(1)-O(1)#2	164.03(18)	O(6)-Tb(1)-O(1)#2	71.14(19)
O(7)#1-Tb(1)-O(1)#2	118.42(18)	O(4)#1-Tb(1)-O(1)#2	68.23(19)
O(2)#2-Tb(1)-O(1)#2	52.30(18)	O(3)-Tb(1)-O(3)#1	134.56(14)
O(8)-Tb(1)-O(3)#1	65.91(19)	O(2)-Tb(1)-O(3)#1	69.96(17)
O(6)-Tb(1)-O(3)#1	136.38(18)	O(7)#1-Tb(1)-O(3)#1	128.89(17)
O(4)#1-Tb(1)-O(3)#1	51.35(18)	O(2)#2-Tb(1)-O(3)#1	121.9(2)
O(2)#2-Tb(1)-O(3)#1	128.89(17)	O(1)#2-Tb(1)-O(3)#1	111.14(18)

Symmetry transformations used to generate equivalent atoms: # 1 -x+1/2,y-1/2,-z+3/2
#2 -x+1/2,y+1/2,-z+3/2 #3 -x+1/2,-y+5/2,-z+2

Table S3. Calculation of fluorescence quantum yield of complex **1**

Complex **1**			
υ_{00} (cm^{-1})	20367	A_{00}	330.457
υ_{01} (cm^{-1})	18349	A_{01}	50
υ_{02} (cm^{-1})	17007	A_{02}	189.659
υ_{03} (cm^{-1})	16155	A_{03}	179.857
I_{01} (a.u)	5101	**Ar**	**749.973**
I_{02} (a.u)	37420	τ **(ms)**	**0.880**
I_{02}/I_{01}	7.336	**1/τ**	**1.136**
η**%**		**66.0**	

Table S4. Comparison of literature reports for CPs as sensors of Pb^{2+}

Complexes	K_{sv} (M^{-1})	Detection Limit	On - Off Response	Medium	Ref.
$[Ln_2(FDC)_3DMA(H_2O)_3]DMA_4.5H_2O$	2.97×10^6	8.22×10^{-6}M	Turn-on	H_2O	1
Tb-1	/	3.43×10^{-6}M	Turn-on	acetonitrile	2
MOF-5	/	0.2×10^{-7}M	Turn-on	H_2O	3
$[Tb(L)(H_2O)_5]_n$	1.75×10^4	0.7×10^{-7}M	Turn-on	H_2O	4
$[Tb(ppda)(npdc)_{0.5}(H_2O)_2]_n$ **(1)**	1.05×10^5	9.44×10^{-5}M	Turn-on	H_2O	This work

Table S5. Comparison of literature reports for CPs as sensors of $Cr_2O_7^{2-}$

Complexes	K_{sv} (M^{-1})	Detection Limit	On - Off Response	Medium	Ref.
$[Eu(Hpzbc)_2(NO_3)]\cdot H_2O$	/	2.2×10^{-5}M	Turn-off	ethanol	5
$\{[Tb(TATAB)(H_2O)_2]\cdot NMP\cdot H_2O\}n$	1.11×10^4	1.0×10^{-5}M	Turn-off	H_2O	6
$[EuL(CH_3COO)Cl]_n$	1.15×10^4	8.63×10^{-5}M	Turn-off	H_2O	7
$\{[Zn_4(Trz)_6(HCOO)_2]\}_n$	9.72×10^3	5.82×10^{-4}M	Turn-off	H_2O	8
$[Zn(L)(H_2L)]_n$	1.89×10^3	1.14×10^{-5}M	Turn-off	H_2O	9
$[Eu(Hmcd)(H_2O)(DMF)_2]_n$	2.91×10^3	1.34×10^{-5}M	Turn-off	H_2O	10
$[Tb(ppda)(npdc)_{0.5}(H_2O)_2]_n$ **(1)**	4.97×10^6	6.00×10^{-5}M	Turn-off	H_2O	This work

Table S6. Comparison of literature reports for CPs as sensors of PO_4^{3-}

Complexes	K_{sv} (M^{-1})	Detection Limit	On - Off Response	Medium	Ref.
$\{[Eu(bcpt)(HCOO)]\cdot 0.5H_2O\}_n$	1.27×10^4	2.74×10^{-4}M	Turn-off	H_2O	11
$[Ln(DLDA)(DMF)(H_2O)(COO)]_n$	1.82×10^3	1.88×10^{-5}M	Turn-off	H_2O	12
$\{[Zn_4(L^{3-})_2(O^{2-})(H_2O)_2]\cdot 4EtOH\}_n$	3.69×10^4	0.1×10^{-6}M	Turn-off	H_2O	13
$[(CH_3)_2NH_2]_6[M_6(OBA)_6(L_1)_3(SO_4)_2]\cdot SO_4\cdot x$	6.99×10^3	6.5×10^{-6}M	Turn-off	H_2O	14
$[Tb(ppda)(npdc)_{0.5}(H_2O)_2]_n$ **(1)**	4.48×10^4	1.01×10^{-5}M	Turn-off	H_2O	This work

Table S7. Comparison of literature reports for CPs as sensors of Tyr

Complexes	K_{sv} (M^{-1})	Detection Limit	On - Off Response	Medium	Ref.
$[Zr_6O_4(OH)_8(H_2O)_4(L)_2]·8DMF·10H_2O$	3.75×10^5	9.40×10^{-8}M	Turn-off	H_2O	15
$[Tb(ppda)(npdc)_{0.5}(H_2O)_2]_n$ **(1)**	4.81×10^5	1.43×10^{-5}M	Turn-off	H_2O	This work

Table S8. Comparison of literature reports for MOFs as sensors of Trp

Complexes	K_{sv} (M^{-1})	Detection Limit	On - Off Response	Medium	Ref.
Cu-MOF-modified	/	5.46×10^{-5} M	Turn-on	H_2O	16
Zn-Hbtc-BPY/Tb^{3+}	/	3.10×10^{-6}M	Turn-on	H_2O	17
$[Zn_4(pta)_3(H_2O)_{1.5}]$	/	4.29×10^{-8}M	Turn-on	H_2O	18
$[La(L_2)(H_2O)]$·solvent	1.69×10^3	1.67×10^{-4}M	Turn-off	H_2O	19
$[Tb(ppda)(npdc)_{0.5}(H_2O)_2]_n$ **(1)**	2.60×10^5	6.99×10^{-5}M	Turn-on	H_2O	This work

Table S9. Calculation results of singlet state energy level and the corresponding wavelength of excitation light of selected amino acids.

Amino acids	Singlet state energy level (eV)	Excitation light wavelength (nm)
Alanine	5.2382	236.69
Arginine	5.2456	236.36
Asparagine	5.1484	240.82
Aspartic Acid	5.2749	235.04
Cysteine	5.1767	239.50
Glutamine	5.3442	232.00
Glutamic Acid	5.3536	231.59
Glycine	5.4098	229.19
Histidine	4.6439	266.98
Isoleucine	5.3979	229.69
Leucine	5.2784	234.89
Lysine	5.4104	229.16
Methionine	5.3779	230.54
Phenylalanine	4.9072	252.66
Proline	5.1332	241.54
Serine	5.2474	236.28
Threonine	5.2171	237.65
L-Tryptophan	**4.3051**	**287.99**
D-Tryptophan	4.3527	284.84
Tyrosine	4.8780	254.17
Valine	5.3902	230.02
H_2npdc	**3.8111**	**326.01**

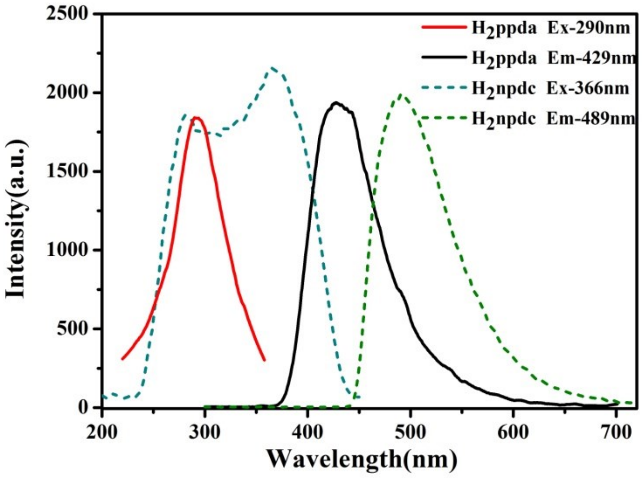

Fig. S1 The PL spectra of H_2ppda (solid line) and H_2npdc ligand (dotted line).

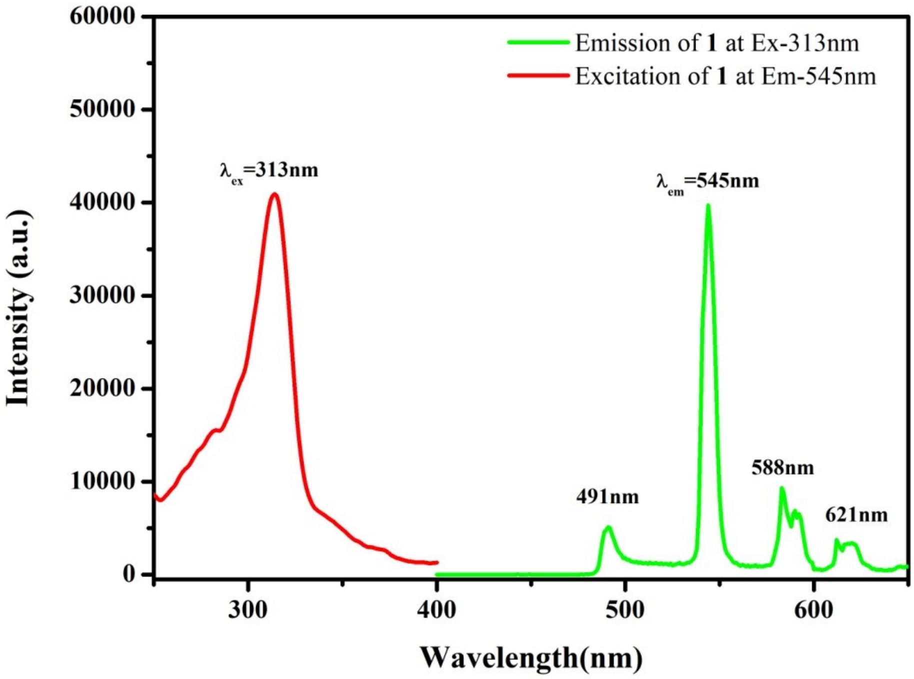

Fig. S2 Solid state excitation and emission spectra of compond **1** at room temperature.

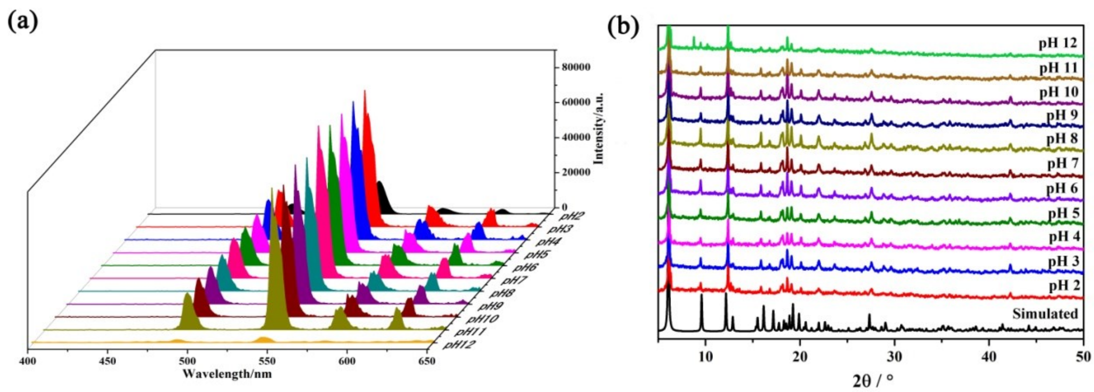

Fig. S3 (a) The emission spectrum of compond **1** dispersed in pH aqueous solutions (pH=2-12). (b) The PXRD patterns of **1** dispersed in pH aqueous solutions.

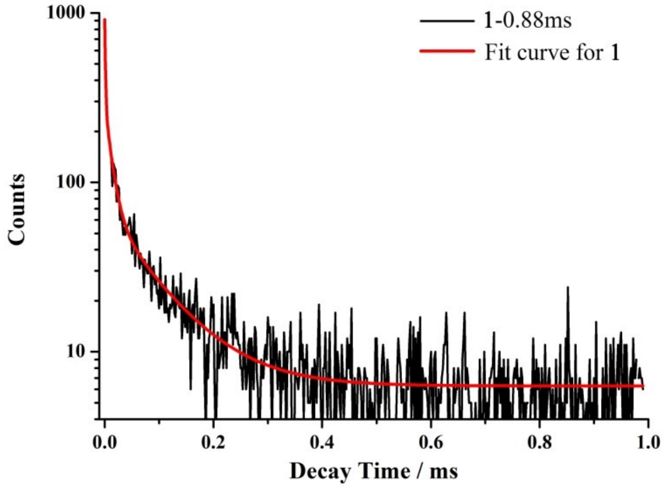

Fig. S4 The fluorescence decay and fit curve for **1**

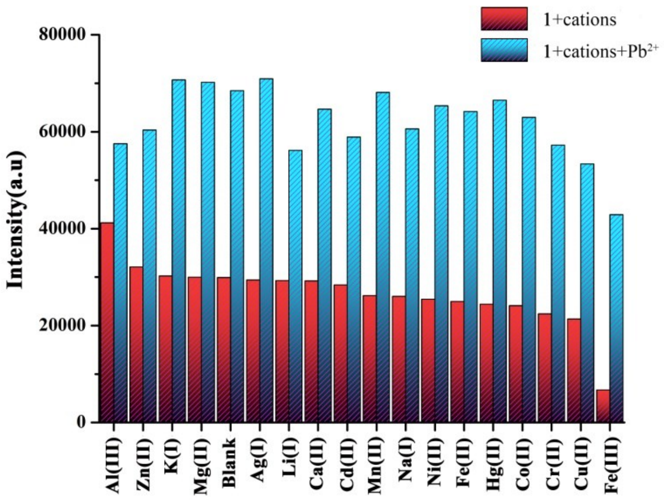

Fig. S5 Comparison of fluorescence intensity of **1** in various cations aqueous solutions and after addition of 300μL Pb^{2+}.

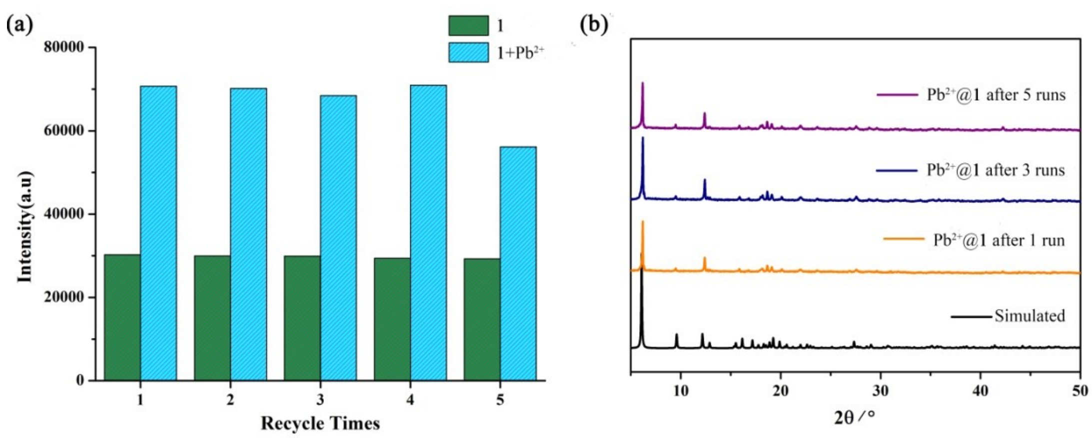

Fig. S6 (a) Enhancing and recovery test of **1** in $Pb(NO_3)_2$ aqueous solutions. (b) PXRD patterns of

1 after five recles.

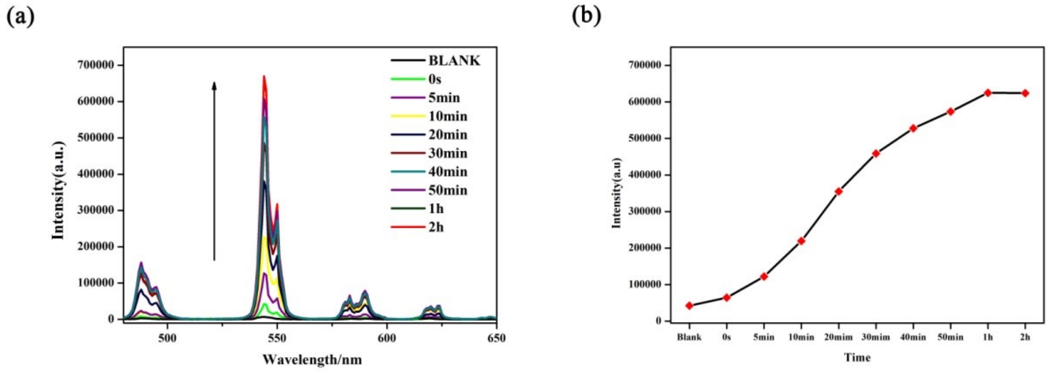

Fig. S7 (a) Time-dependent emission spectra fort **1** detecting Pb^{2+} ions. (b)The curve for fluorescence intensity of **1** versus time after addition of 300 μL of Pb^{2+} ions.

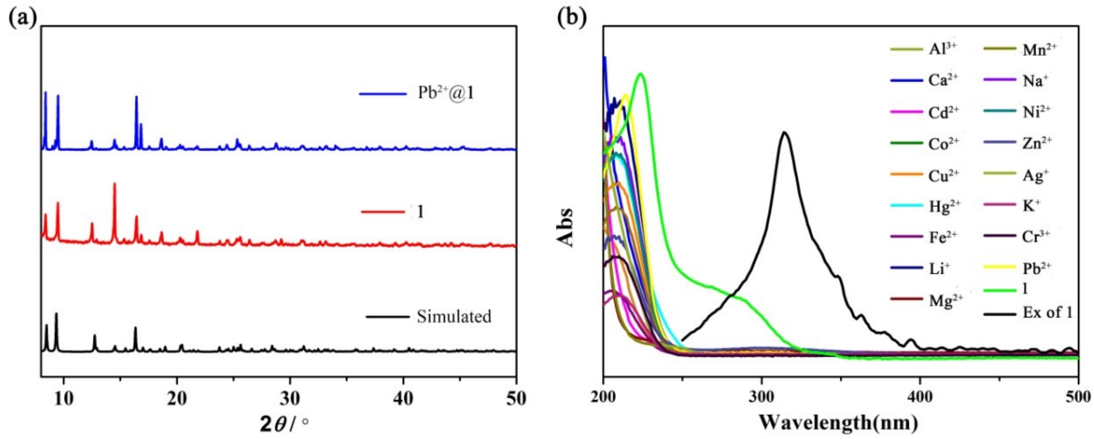

Fig. S8 (a) PXRD patterns of **1** and **1** soaked in $Pb(NO_3)_2$ aqueous solutions; (b) the UV-Vis adsorption spectra of **1**, various cations and the excitation spectrum of **1**.

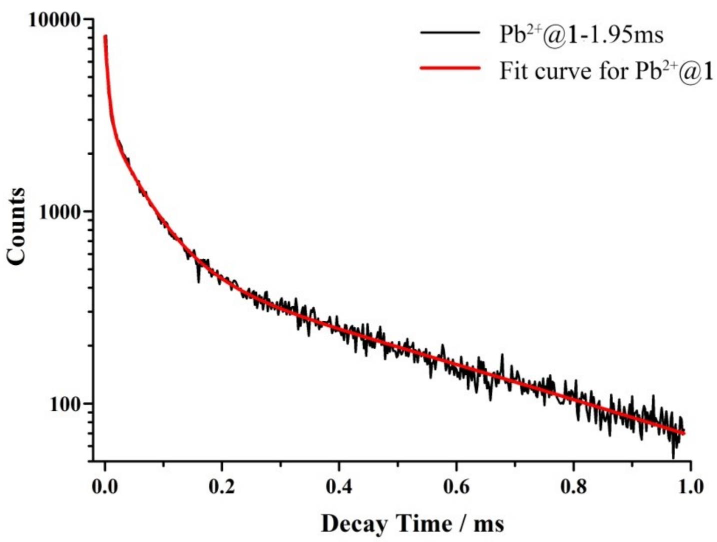

Fig. S9 The fluorescence decay and fit profiles of Pb^{2+}@**1**.

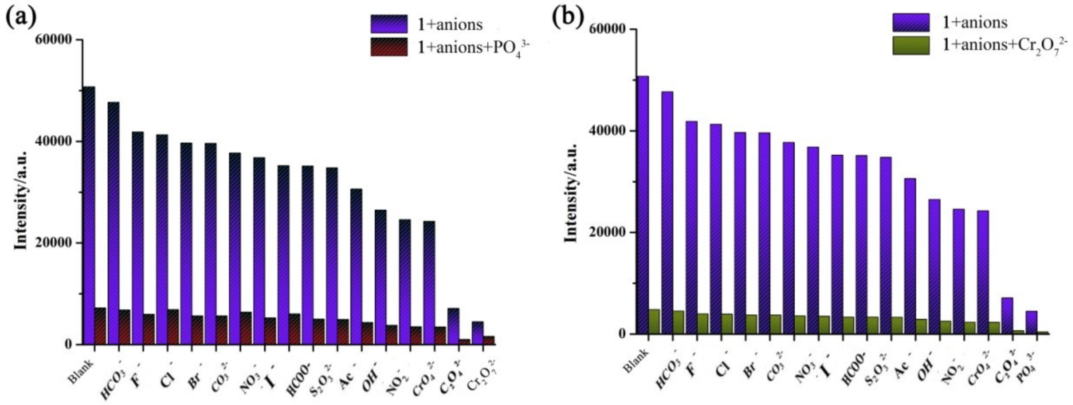

Fig. S10 Fluorescence intensity histogram of **1** in different anions and mixed anions, (a) for PO_4^{3-} ions and (b) for CrO_7^{2-} ions.

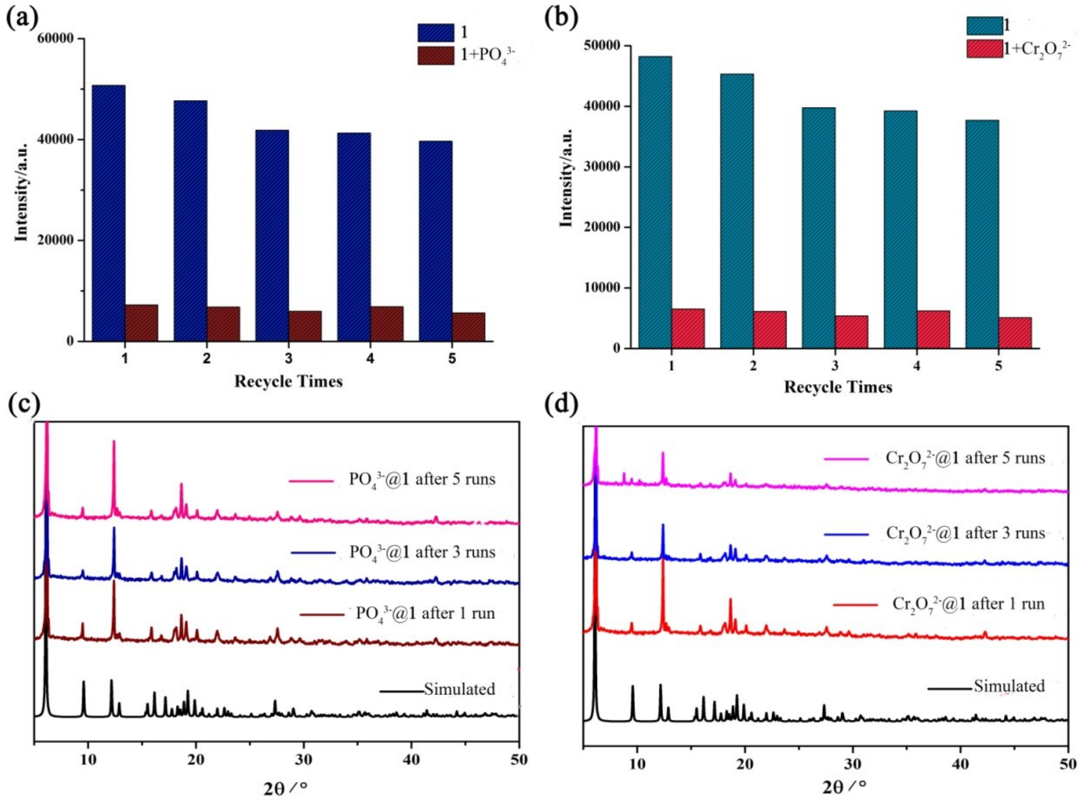

Fig. S11 (a) Quenching and recovery test of **1** detecting PO_4^{3-} ions. (b) Quenching and recovery test of **1** detecting $Cr_2O_7^{2-}$ ions. (c) and (d) PXRD patterns after recovery test.

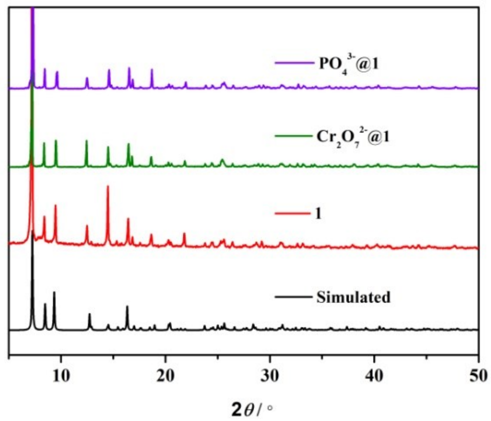

Fig. S12 PXRD patterns of **1** and **1** soaked in PO_4^{3-} or $Cr_2O_7^{2-}$ aqueous solutions.

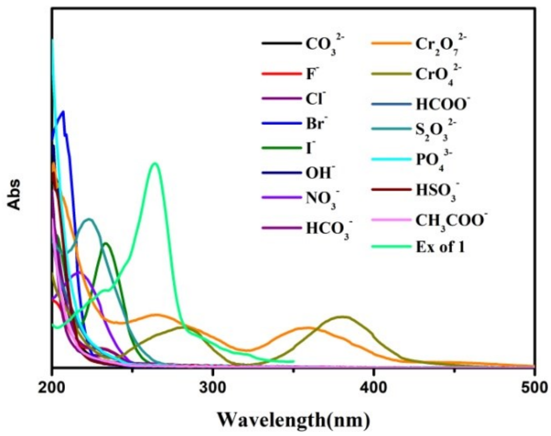

Fig. S13 the UV-Vis adsorption spectra of various anions and the excitation spectrum of **1**.

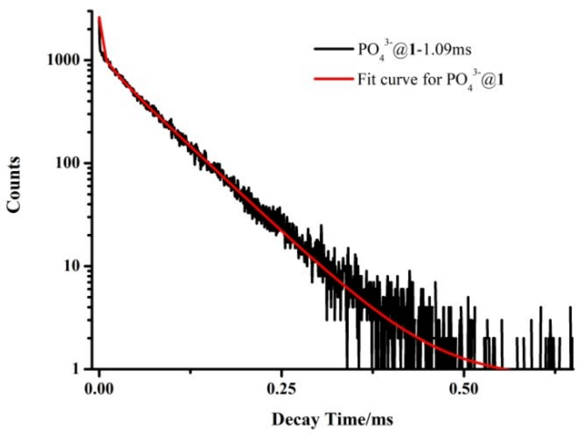

Fig. S14 The fluorescence decay and fit profiles of PO_4^{3-}@**1**.

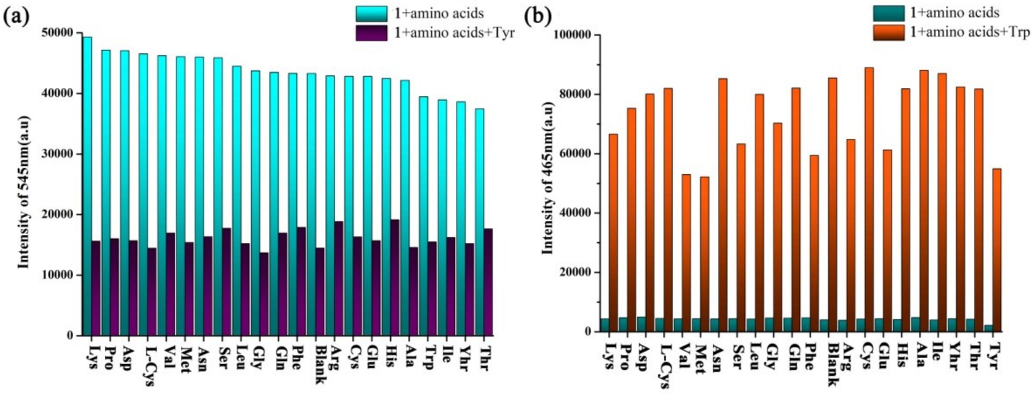

Fig. S15 (a) Comparison of fluorescence intensity of **1** at 545nm in different amino acids solutions and after addition of Tyr. (b) Comparison of fluorescence intensity of **1** at 465nm in different amino acids slolutions and after addition of Trp.

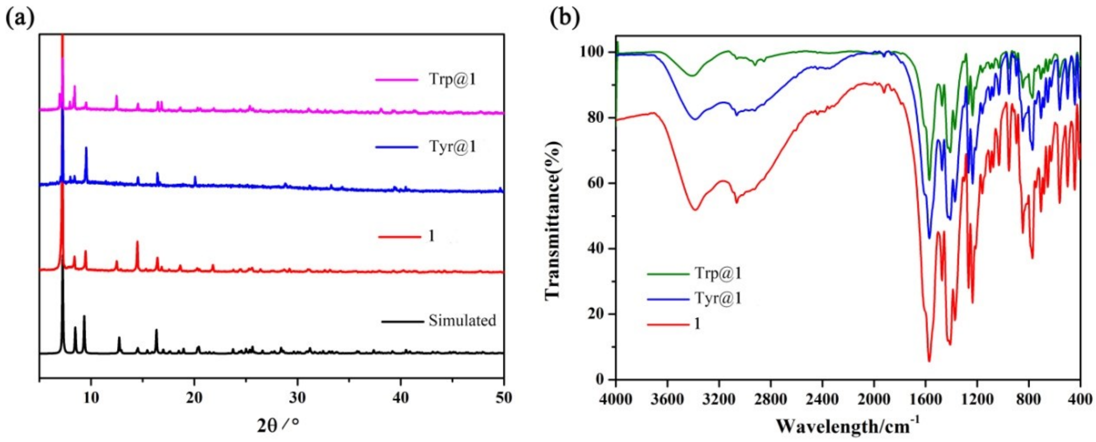

Fig. S16 (a) PXRD patterns of **1** and **1** immersed in Tyr or Trp. (b) FTIR spectra of Tyr@ **1** and Trp@ **1.**

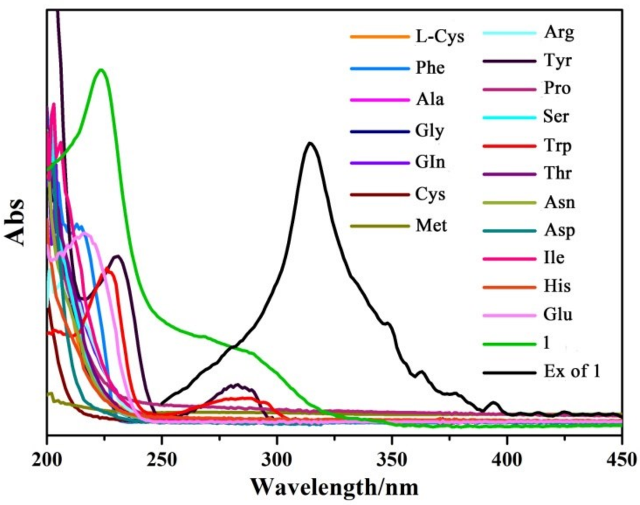

Fig. S17 The adsorption spectra of various amino acids and **1**, and the excitation spectrum of **1**.

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