Electronic Supplementary Information (ESI)

A stable Zn-MOF multifunctional fluorescent probe was used for the specific detection of Fe^{3+}, $V_2O_7^{4-}$, *p*-nitrotoluene

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Materials and general methods

All chemicals were commercially obtained that without further purification. $Zn(NO_3)_2{\cdot}6H_2O$, H_2bpdc and Htpba were purchased by Jinan Henghua Sci. & Tec. Co., Ltd. Powder X-ray diffraction was carried out on a Bruker SMART APEX II CCD X-ray single crystal diffractometer. Thermogravimetric analysis (TGA) was performed by a Trisch STA409pc analyzer under a nitrogen atmosphere. Luminescence spectra were recorded on an FLS 920 fluorescence analyzer. Infrared spectra were recorded on VERTEX70. The UV-VIS spectrum was recorded by a UV-vis spectrophotometer.

X-Ray crystallography

Crystallographic data for **1** was collected on a Bruker Smart 1000 diffractometer equipped with graphite-monochromatic Cu Kα radiation ($\lambda = 0.71073$ Å) using the ω-scan technique at room temperature. Semiempirical absorption corrections were applied using the SADABS

program. The structure was solved by direct methods using SHELXS-2018 and was refined by full matrix leastsquares on $|F|^2$ using the SHELXTL-2018 program. All non-hydrogen atoms were refined anisotropically. The organic hydrogen atoms were geometrically generated, the hydrogen atoms of water molecules were located from difference Fourier maps and were refined with the common isotropic thermal parameter. Details of the crystal parameter data collection and refinement for **1** are summarized in Supplementary Table S1.

Luminescence sensing experiments

Fully ground 1.65 mg of **1** was added to 2.7 mL deionized water and sonicated for 30 min to make it fully dispersed. Then 300 μL of different analytes with a concentration of 1.0×10^{-3} M were added to the suspension for fluorescence test.

Table S1 The crystal data for **1**.

Compound	**1**
Formula	$C_{32}H_{19}N_4O_4Zn$
Formula Weight	588.88
T/K	273.15
Crystal System	triclinic
Space Group	$P\bar{1}$
a (Å)	10.4776(4)
b (Å)	11.3099(4)
c (Å)	11.4836(4)
α (°)	75.2050(10)
β (°)	73.4410(10)
γ (°)	73.7360(10)
V (A^3)	1229.18(8)
Z	2
D calc.(g cm^{-3})	1.591

μ (mm^{-1})	1.049
F (000)	602
Rint	0.0199
GOOF	1.037
R_1[a]	0.0280
ωR_2[b] [I > 2σ(I)]	0.0707
R_1 (all data)	0.0336
ωR_2 (all data)	0.0734
Largest difference in peak and hole (e $Å^{-3}$)	0.287 -0.237

[a] $R_1 = \Sigma||F_o| - |F_c||/ \Sigma|F_o|$. [b] $\omega R_2 = [\Sigma[\omega(F_o^2-F_c^2)^2]/ \Sigma\omega(F_o^2)^2]^{1/2}$.

Table S2 The performances of different CPs sensors with detecting Fe^{3+} ion.

Fluorescent probes	Detection limit	Ref
$\{[Cd_3(itp)_2(btc)_2]\cdot 4H_2O\}_n$	0.12 μM	(1)
metallosupramolecular polypseudorotaxane	0.893 nM	(2)
ZSTU-1	63.8 nM	(3)
$TbL_{0.5}(H_2L)_{0.5}(H_2O)$ DMF	0.7 μM	(4)
CP **1**	1.72 μmol/L	(5)
$\{[Zn_3(mtrb)_3(btc)_2]\cdot 3H_2O\}_n$	1.78 μM	(6)
TPA-Bp	1.02×10^{-5} M	(7)
Sr_2(tcbpe)	0.14 mM	(8)
This work	9.33 nM	

Table S3 The performances of different CPs sensors with detecting *p*-nitrotoluene.

Fluorescent probes	Detection limit	Ref
$[Cd_4(bptc)_2(DMA)_4(H_2O)_2\cdot 4DMA]$	0.37 ppm	(9)
CP **4**	0.88 ppm	(10)
1A and 2A	0.062 μM	(11)
CCH	25×10^{-9} M	(12)
GCE/a-MnO_2	144 nM	(13)
AIEgens	39ppb	(14)
This work	50.9 nM	

Table S4 HOMO and LUMO energies calculated for nitroaromatic explosives at B3LYP/6-31G** level of theory.

Analytes	HOMO (eV)	LUMO (eV)	Band gap (eV)
Htpba	-6.4028	-1.9524	4.4504
H_2bqdc	-6.5957	-2.6253	3.9704
NB[15]	-7.5912	-2.4283	5.1629
TNT[15]	-8.4592	-3.4926	4.9666
1,3-DNB[15]	-7.9855	-3.4311	4.5544
1,3,5-TNB[16]	-8.9338	-3.6831	5.2507
2,4-DNT[15]	-7.7645	-3.2174	4.5471
m-NT[16]	-7.2725	-2.3619	4.9106
o-NT[17]	-7.3511	-2.3015	5.0496
2,4-DNP[18]	-8.00572	-3.77103	4.23469
1,4-DNB[16]	-8.3525	-3.4967	4.8557
p-NT[19]	-7.362160	-2.320531	5.041628

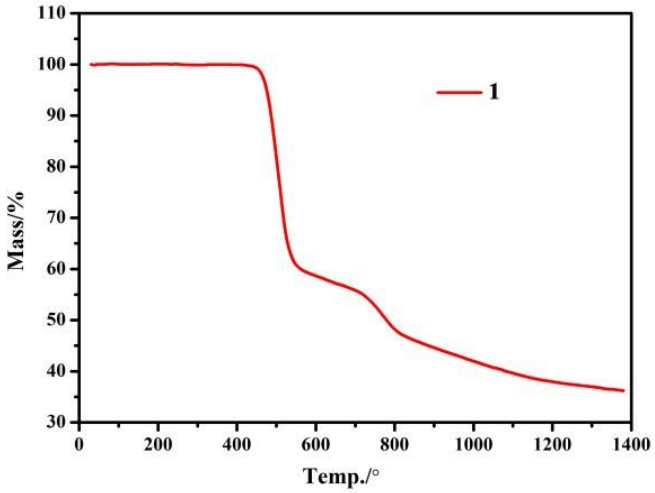

Fig.S1 TG analysis plots of complex **1**.

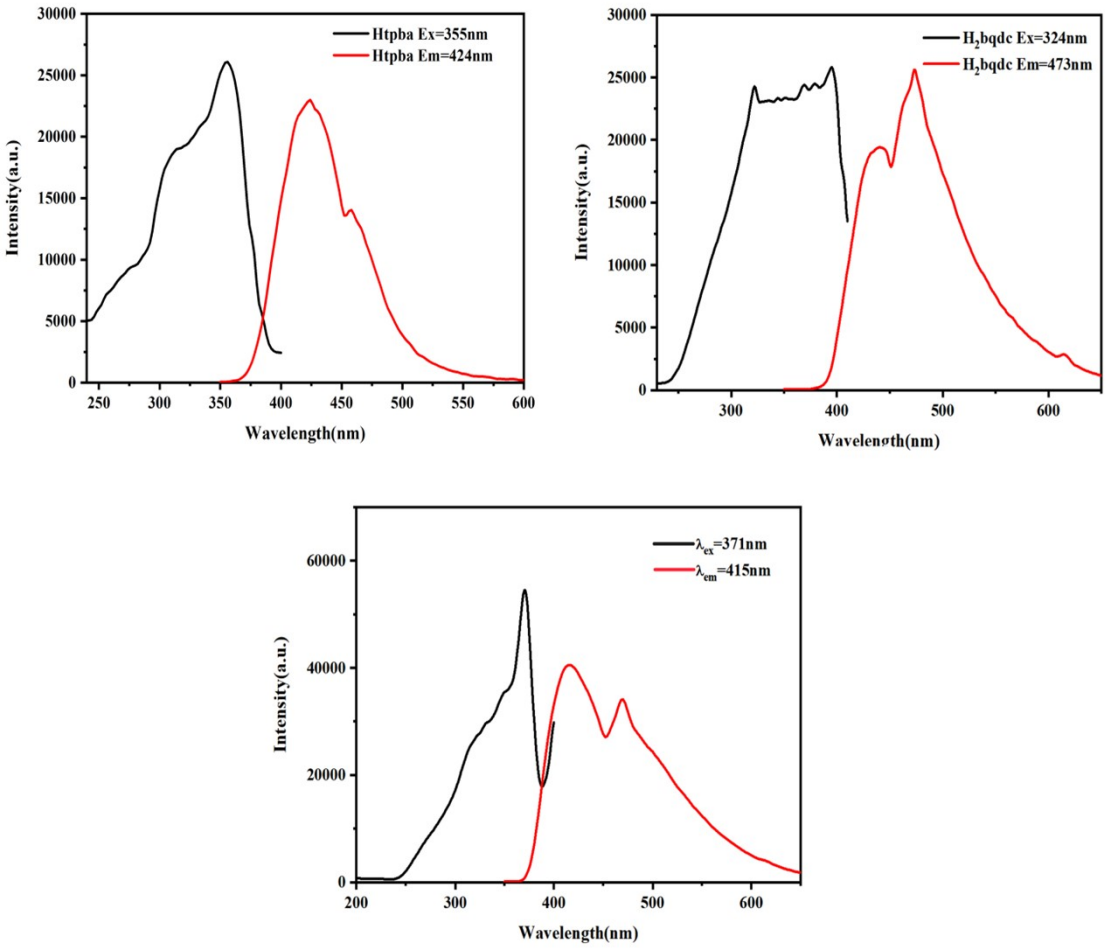

Fig.S2 Excitation and emission spectra of (a) H_2bqdc ligand; (b) ligand Htpba and (c) complex **1** at the room temperature.

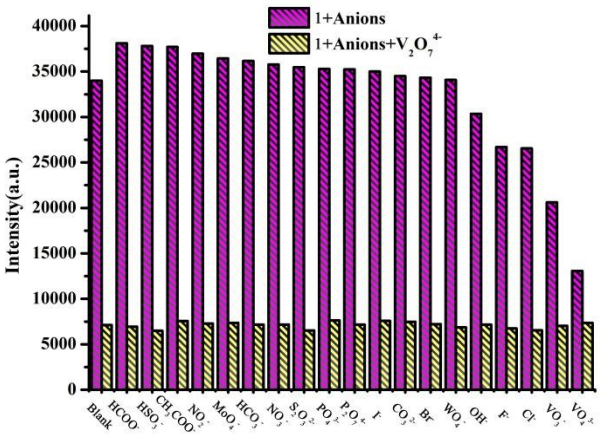

Fig.S3 Comparison of fluorescence intensity of complex **1** in aqueous solution with different interfering cations and in aqueous solution with equal amount of $V_2O_7^{4-}$.

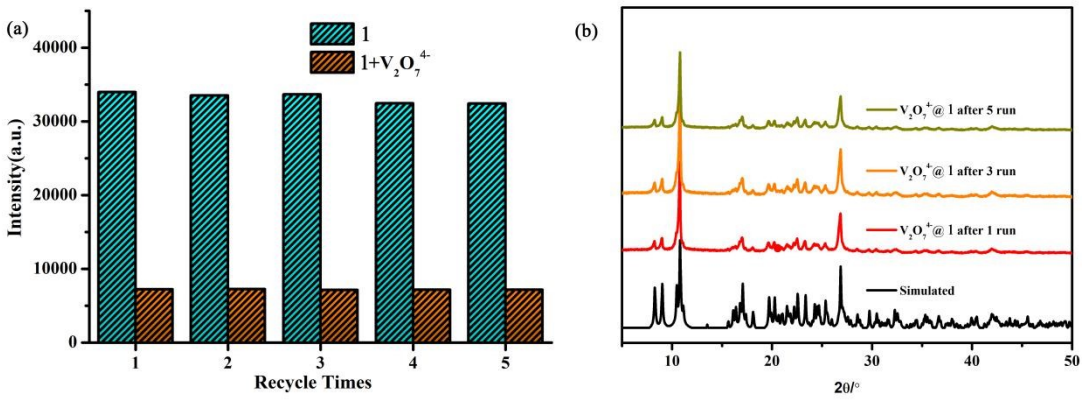

Fig.S4 (a) Recyclability of complex **1** immerses in $V_2O_7^{4-}$; (b) PXRD patterns of complex **1** after sensing five times.

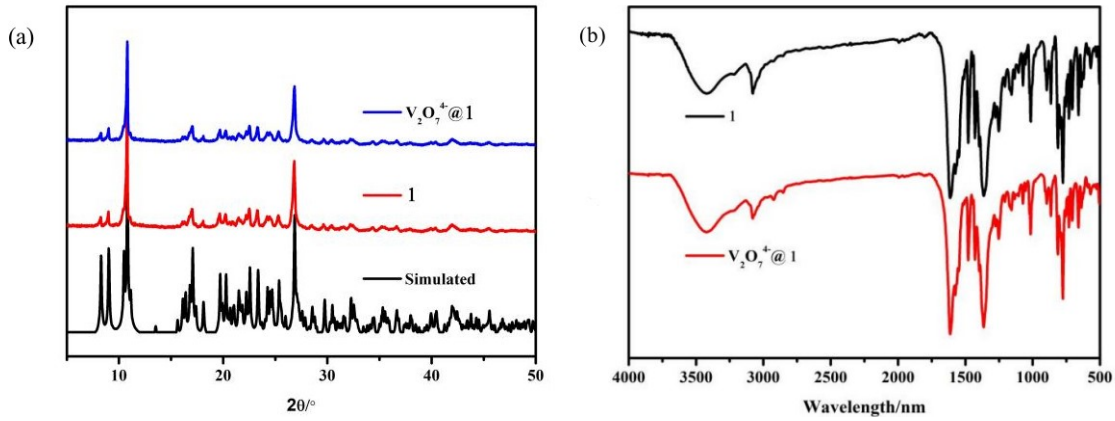

Fig.S5 (a)The PXRD patterns of **1** and $V_2O_7^{4-}$@**1**; (b) The IR spectra of **1**, **1** soaked in $V_2O_7^{4-}$ aqueous solutions.

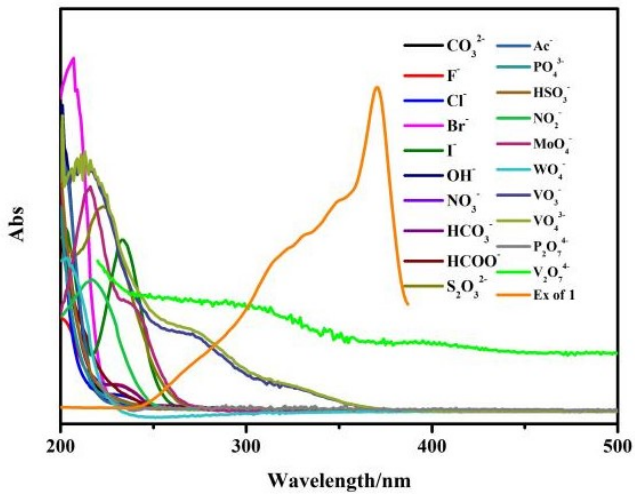

Fig.S6 UV-vis absorption spectra of anions and the excitation one of **1**.

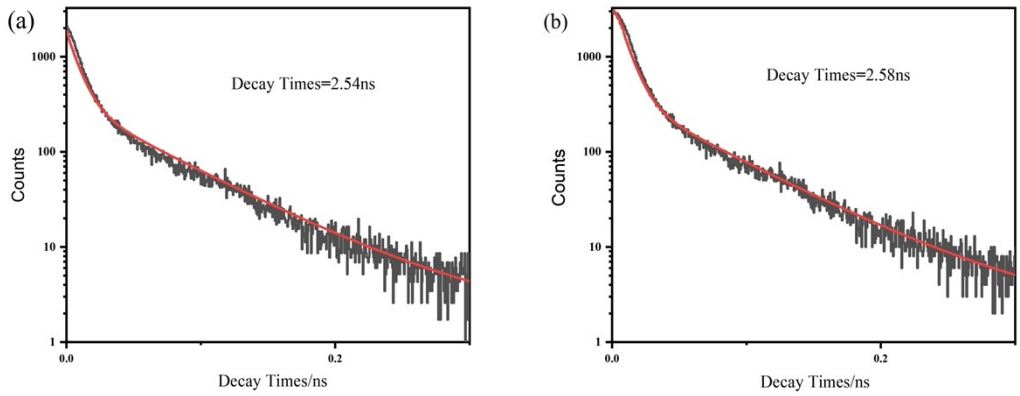

Fig.S7 The fluorescence decay and fit curve for (a) complex **1**; (b) $V_2O_7^{4-}$@**1**.

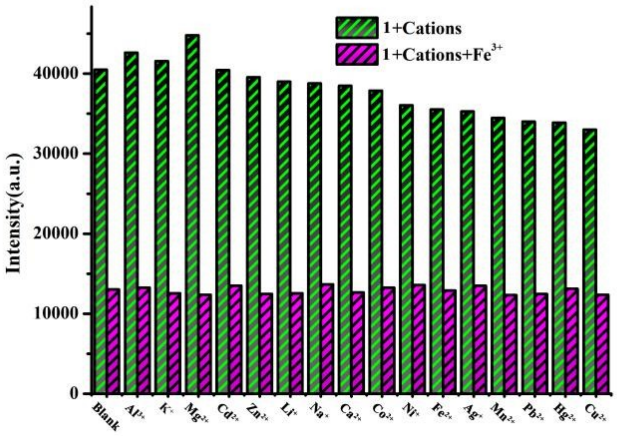

Fig.S8 Comparison of fluorescence intensity of complex **1** in aqueous solution with different interfering cations and in aqueous solution with equal amount of Fe^{3+}.

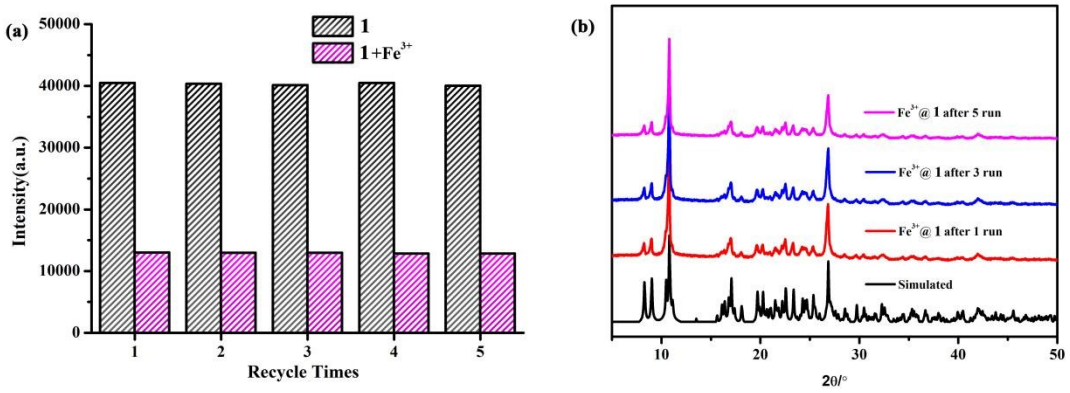

Fig.S9 (a) Recyclability of complex **1** immerses in Fe^{3+}; (b) PXRD patterns of complex **1** after sensing five times.

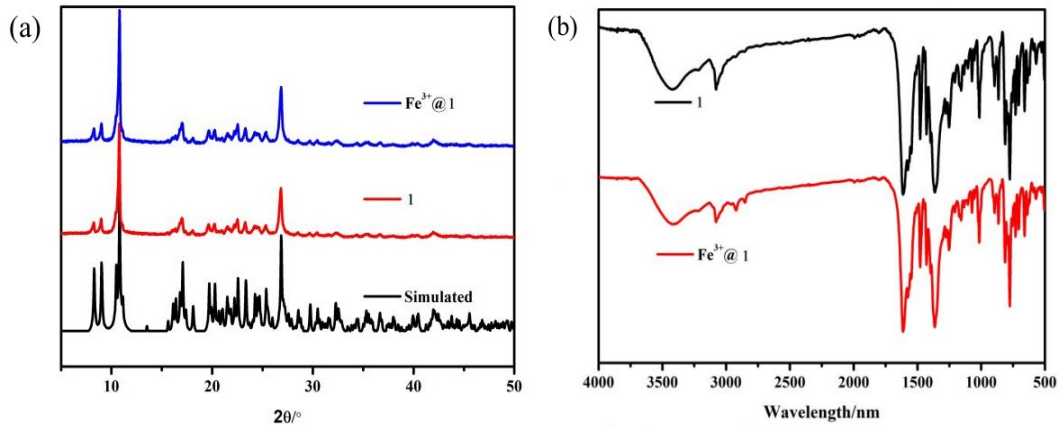

Fig.S10 (a) The PXRD patterns of **1** and Fe^{3+}@**1**; (b) The IR spectra of **1**, **1** soaked in Fe^{3+} aqueous solutions.

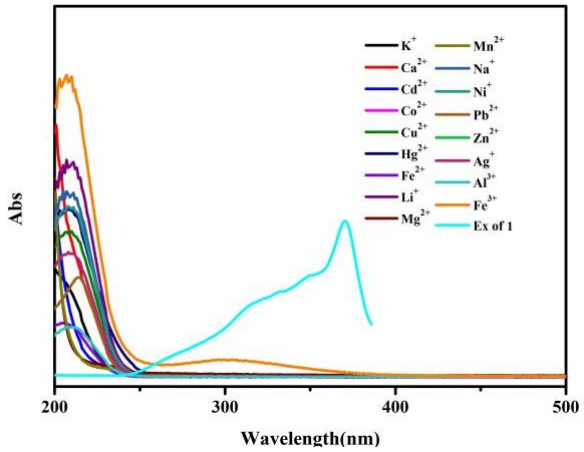

Fig.S11 UV absorption spectra of some cations and the excitation one of **1**.

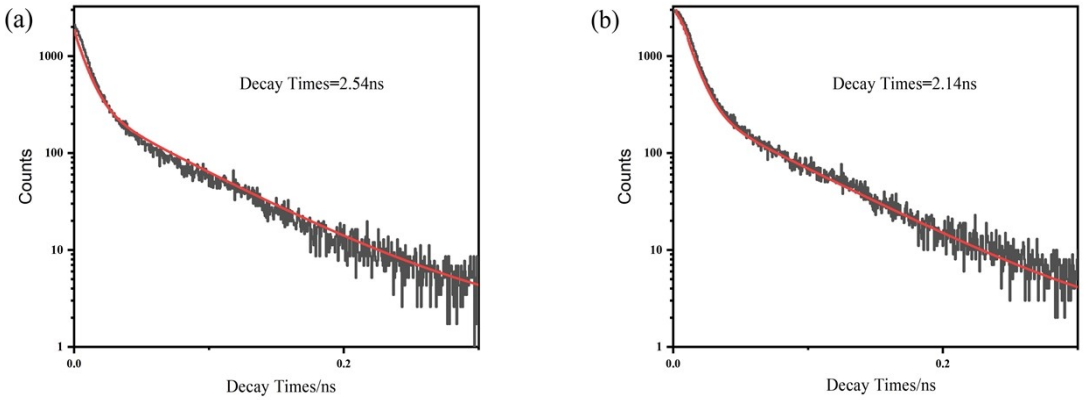

Fig.S12 The fluorescence decay and fit curve for (a) complex **1**; (b) Fe^{3+}@**1**.

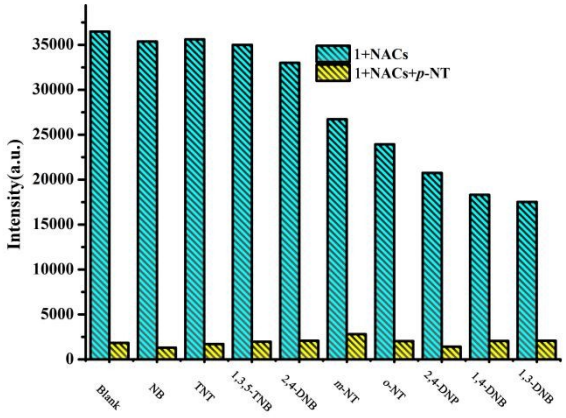

Fig.S13 Comparison of fluorescence intensity of complex **1** in methanol solutions with different interference NACs and the same amount of *p*-NT methanol.

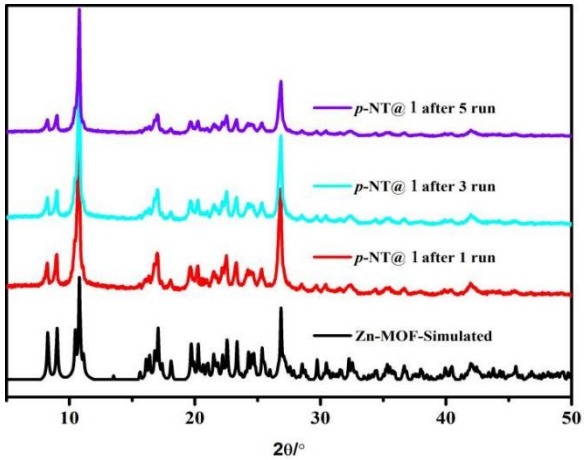

Fig.S14 PXRD patterns of complex **1** after sensing five times.

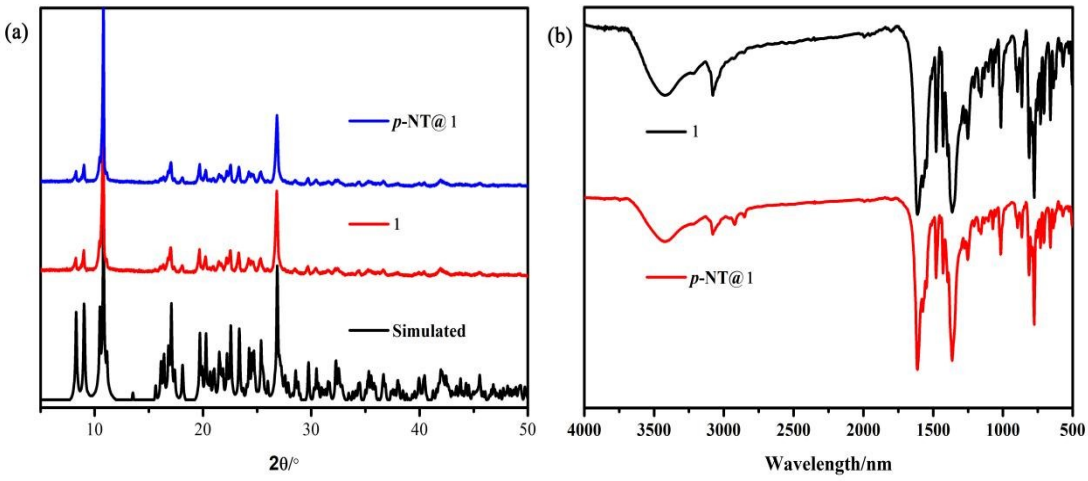

Fig.S15 (a) PXRD of 1 and complex **1** in methanol solution of *p*-NT; (b) IR of *p*-NT@**1** and **1**.

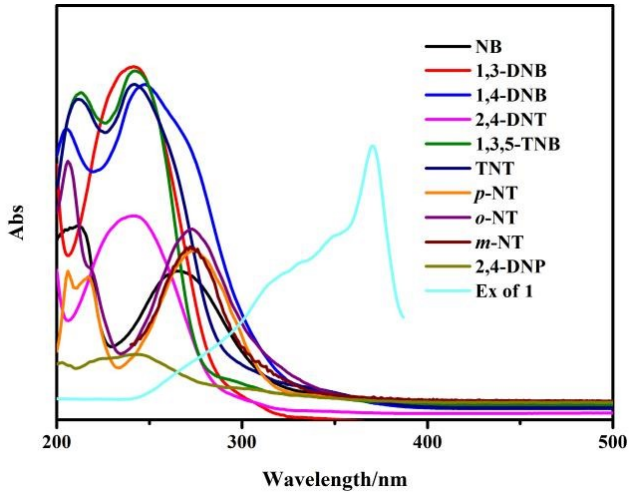

Fig.S16 UV-vis absorption spectrum of NACs and the excitation spectrum of complex **1**.

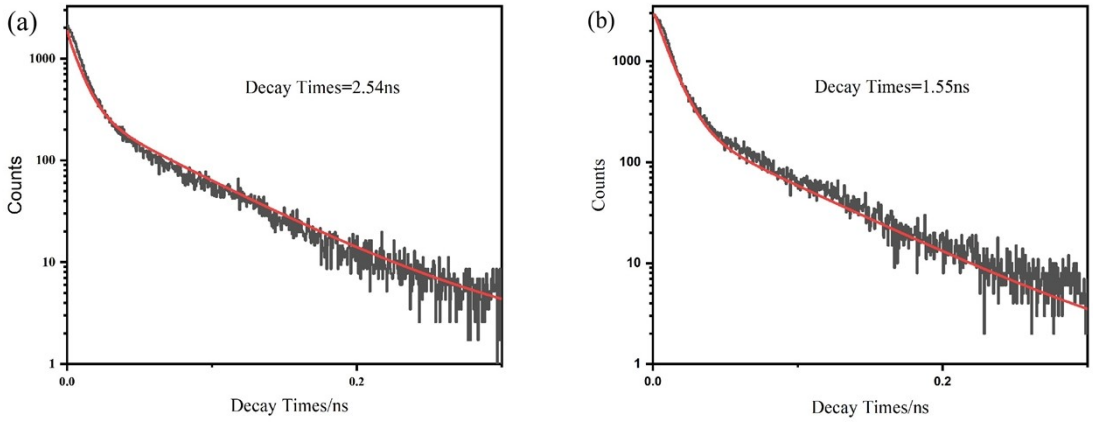

Fig.S17 The fluorescence decay and fit curve for (a) complex **1**; (b) *p*-NT@**1**.

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