Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

A dual-responsive luminescent metal-organic framework as a recyclable luminescent probe for highly effective detecting pyrophosphate and nitrofurantoin

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X-ray Structure Determination

The crystallographic data of the ZTMOF-1 was collected using a Bruker SMARTAPEX CCD diffractometer with MoKa radiation (λ= 0.71073 Å). The crystal structure was successfully solved by the direct method and refined by full-matrix least-squares techniques based on F^2 values with Shelxtl-2014.[1] And the non-hydrogen atoms were refined by anisotropic thermal parameters. The detailed crystallographic data and structure refinement parameters for ZTMOF-1 were summarized in Table S1 and Table S2 in supporting information.

Table S1. Selected bond distances (Å) and angles (°) for ZTMOF-1.

Zn(1)-N(2)#1	2.064(4)	Zn(1)-O(1)	1.965(4)
Zn(1)-O(4)#2	2.020(4)	Zn(1)-N(3)#1	2.141(4)
Zn(1)-N(1)#1	2.175(5)	N(2)-Zn(1)#3	2.064(4)
O(4)-Zn(1)#4	2.020(4)	N(3)-Zn(1)#3	2.141(4)
N(1)-Zn(1)#3	2.175(5)		
N(2)#1-Zn(1)-N(3)#1	76.74(17)	N(2)#1-Zn(1)-N(1)#1	74.90(16)
N(2)#1-Zn(1)-C(21)#2	119.13(17)	O(1)-Zn(1)-N(2)#1	117.22(16)
O(1)-Zn(1)-O(4)#2	94.48(17)	O(1)-Zn(1)-N(3)#1	101.62(18)
O(1)-Zn(1)-N(1)#1	96.57(18)	O(1)-Zn(1)-C(21)#2	123.26(18)
O(4)#2-Zn(1)-N(2)#1	147.40(17)	O(4)#2-Zn(1)-N(3)#1	105.61(18)
O(4)#2-Zn(1)-N(1)#1	95.16(17)	O(4)#2-Zn(1) C(21)#2	28.79(16)
N(3)#1-Zn(1)-N(1)#1	151.01(17)	N(3)#1-Zn(1)C(21)#2	96.88(18)
N(1)#1-Zn(1) C(21)#2	91.68(17)		

Table S2. Crystal data and structure refinements parameters of the ZTMOF-1

Compound	ZTMOF-1
Empirical formula	$C_{23}H_{13}N_3O_4Zn$
Formula weight	460.73
Crystal system	Tetragonal
Space group	I4(1)/acd
a (Å)	29.028(6)
b(Å)	29.028(6)
c(Å)	26.747(8)
α(°)	90
β(°)	90
γ(°)	90
V(Å^3)	22537(12)
Z	32
D_{calc} (g cm^{-3})	1.086
Theta range(°)	3.046-27.552
R(int)	0.0999
GOF on F^2	1.106
R1, wR2 [I > 2σ(I)]	0.0703, 0.2081
R1, wR2 (all data)	0.1232, 0.2424

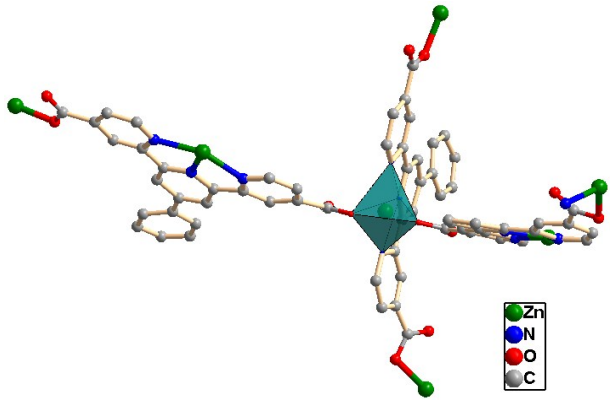


Figure S1. Coordination environment of the Zn^{2+} and ligands. (all the H atoms omitted for clarity.)

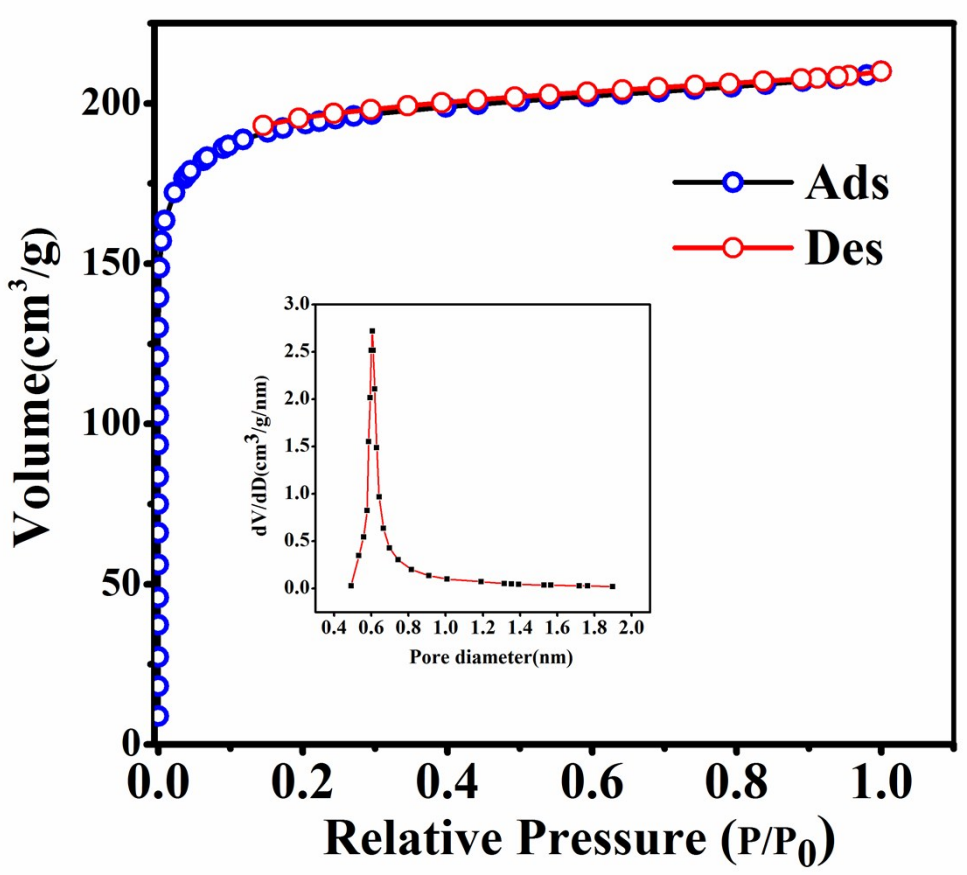


Figure S2:N_2 adsorption/desorption isotherms and pore size distribution of the ZTMOF-1.

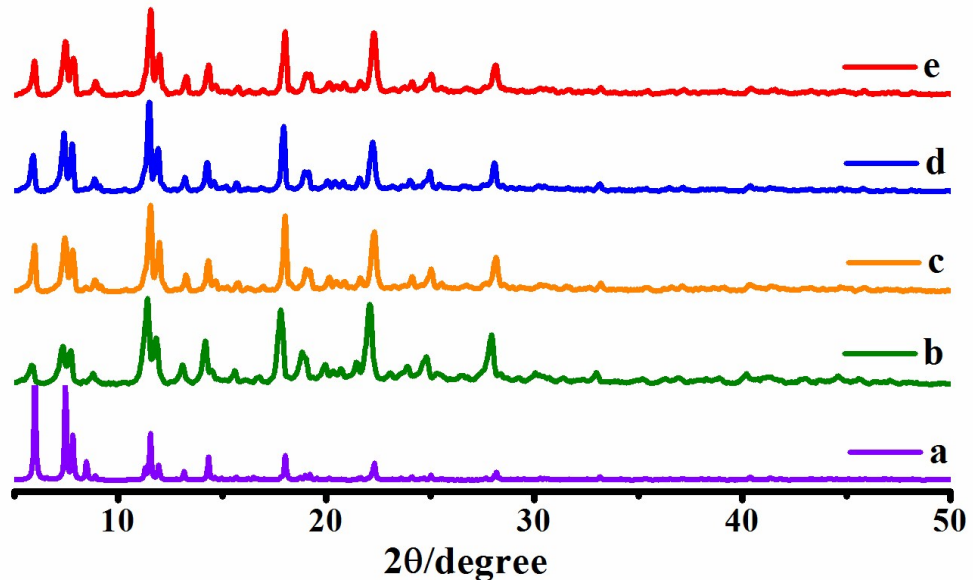


Figure S3. Powder X-ray diffraction(XRD) patterns of ZTMOF-1, (a) the simulated pattern of ZTMOF-1 (b) after immersing in aqueous solution of PPi for 48h (c) after immersing in buffer solution of PPi for 48h (d) after immersing in aqueous solution of nitrofurantoin for 48h.

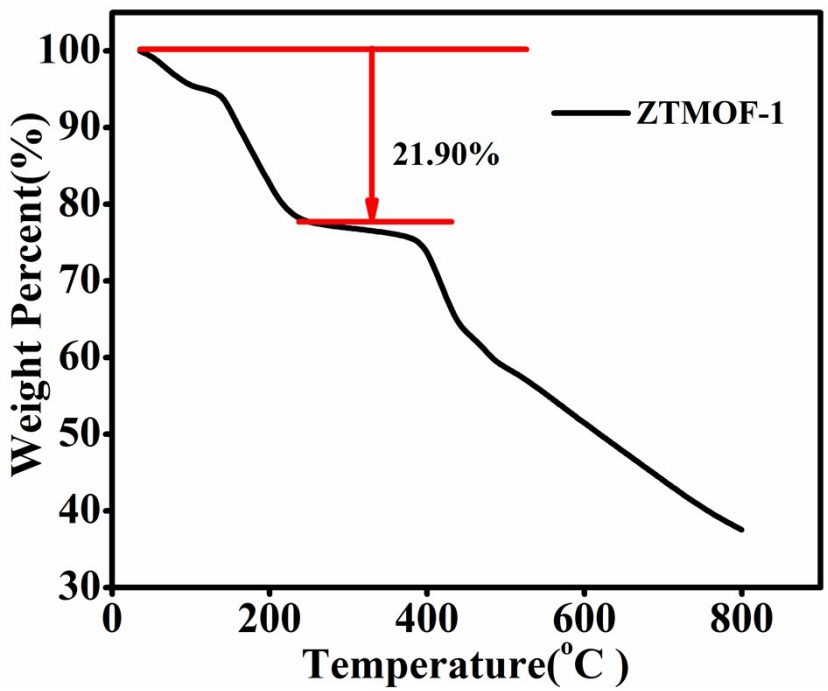


Figure S4. TGA curve of ZTMOF-1.

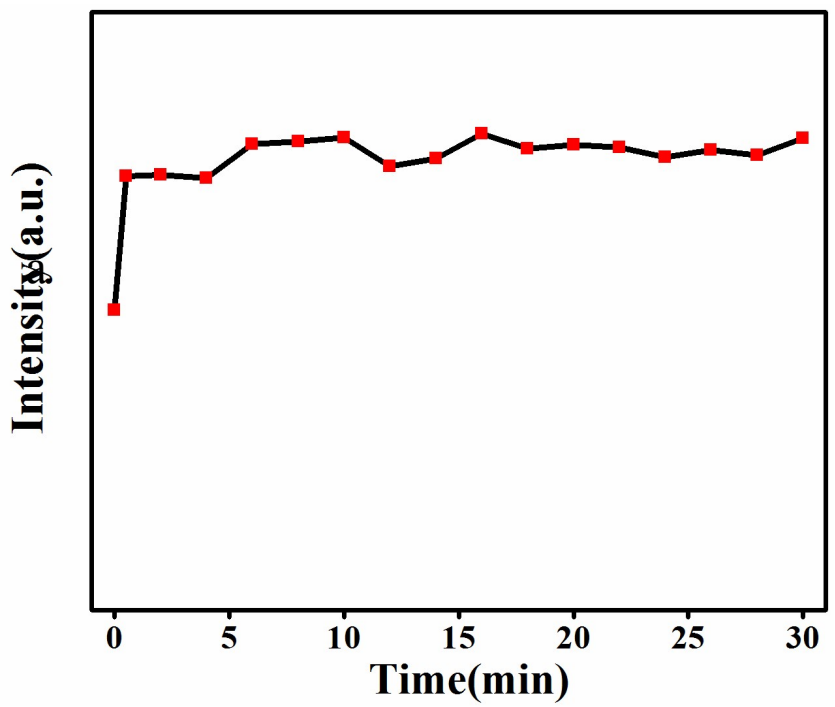
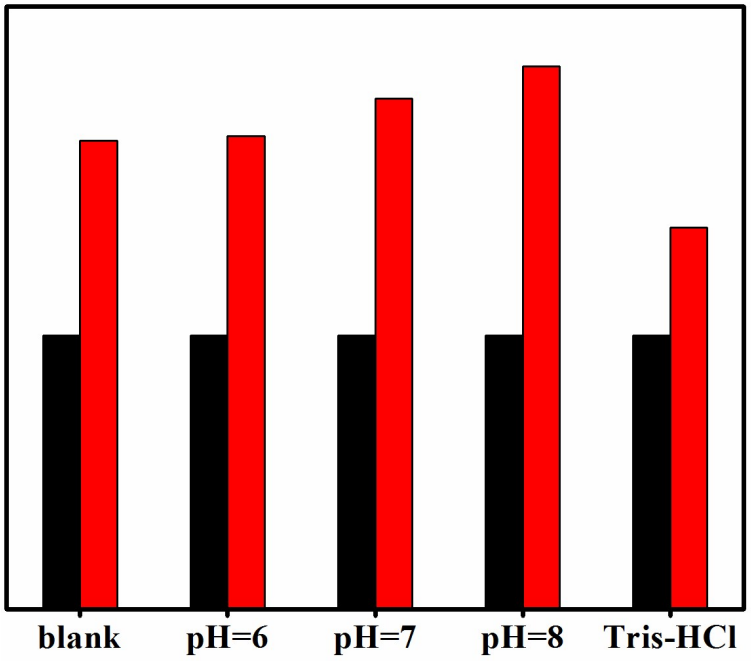


Figure S5: Emission intensity of the ZTMOF-1 at different time.

a



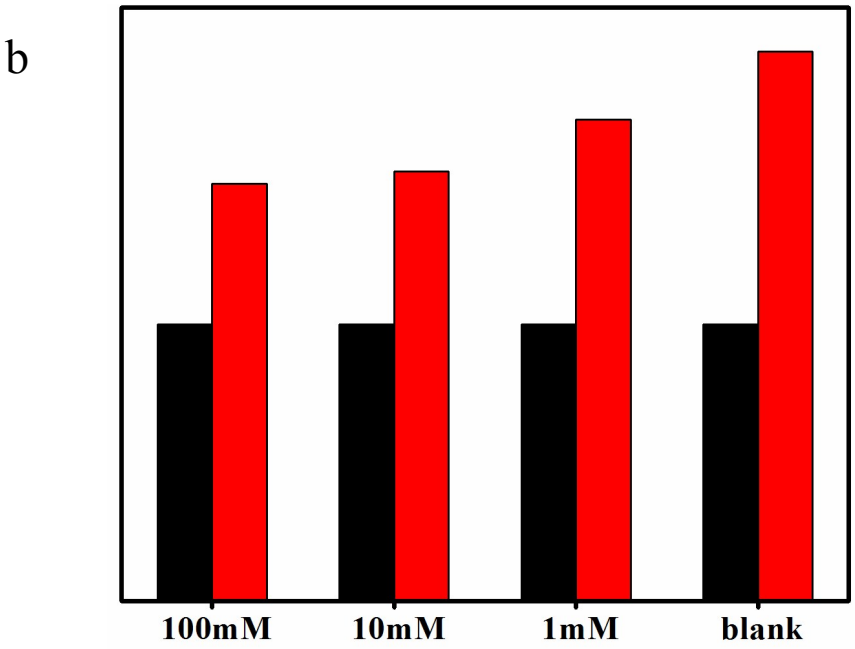


Figure S6. Change of emission intensity of the ZTMOF-1 (a) in aqueous solution with different pH. (b) in Tris-HCl butter solution with different concentrations excitation at 344 nm.

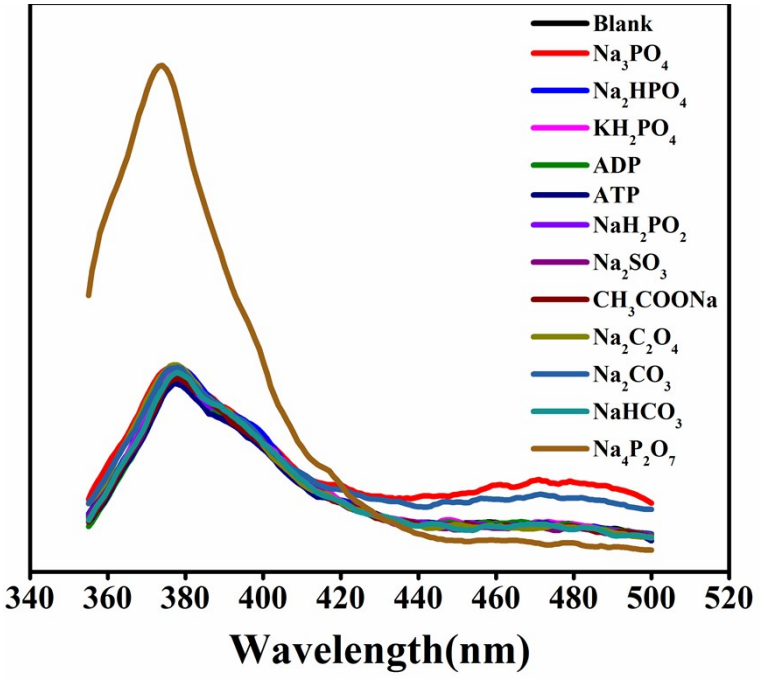


Figure S7. Emission spectra of ZTMOF-1 in different anionic solution (100 μM) excitation at 344 nm.

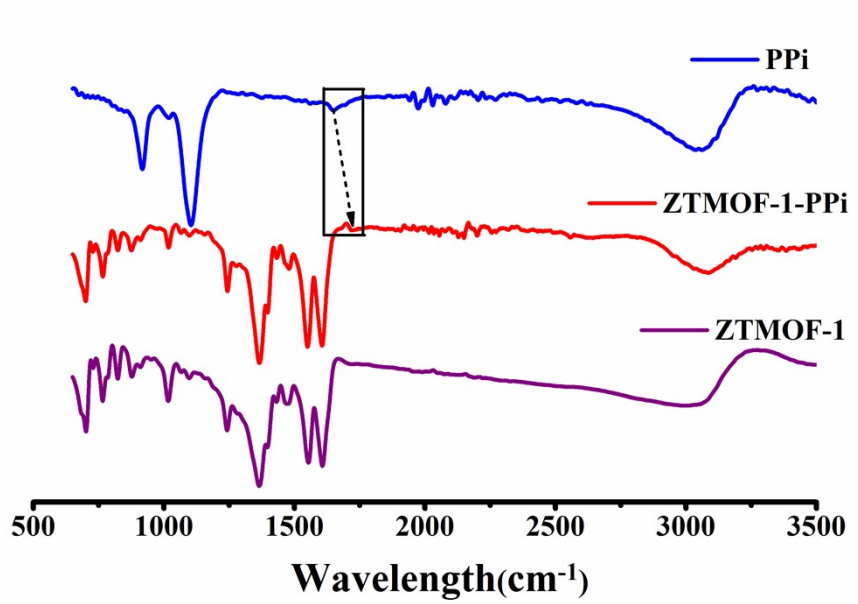


Figure S8 FT-IR spectra of ppi (top), ZTMOF-1(bottom) and ZTMOF-1 treated with PPi (middle).

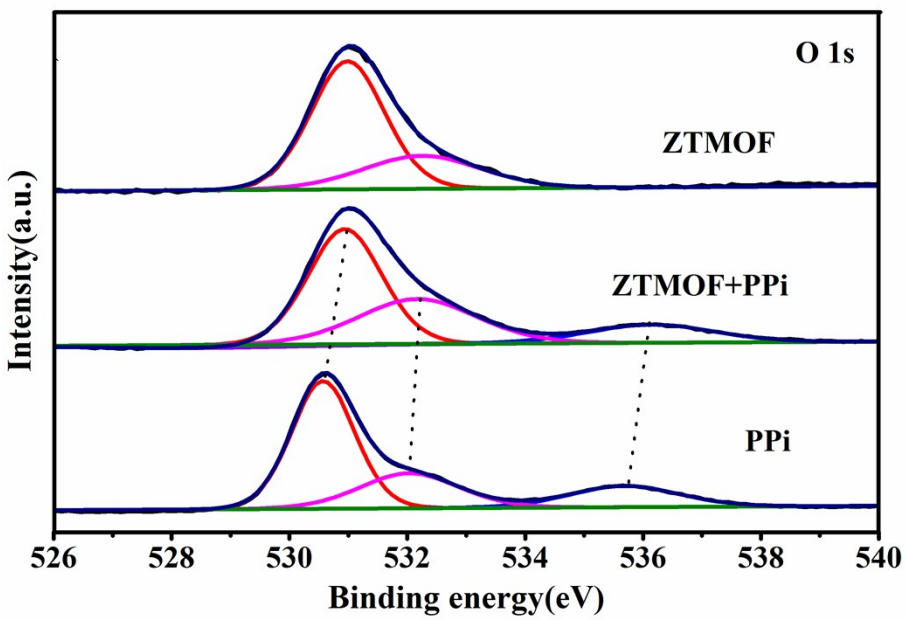


Figure S9. O 1s XPS spectra of ZTMOF, ZTMOF+PPi and PPi.

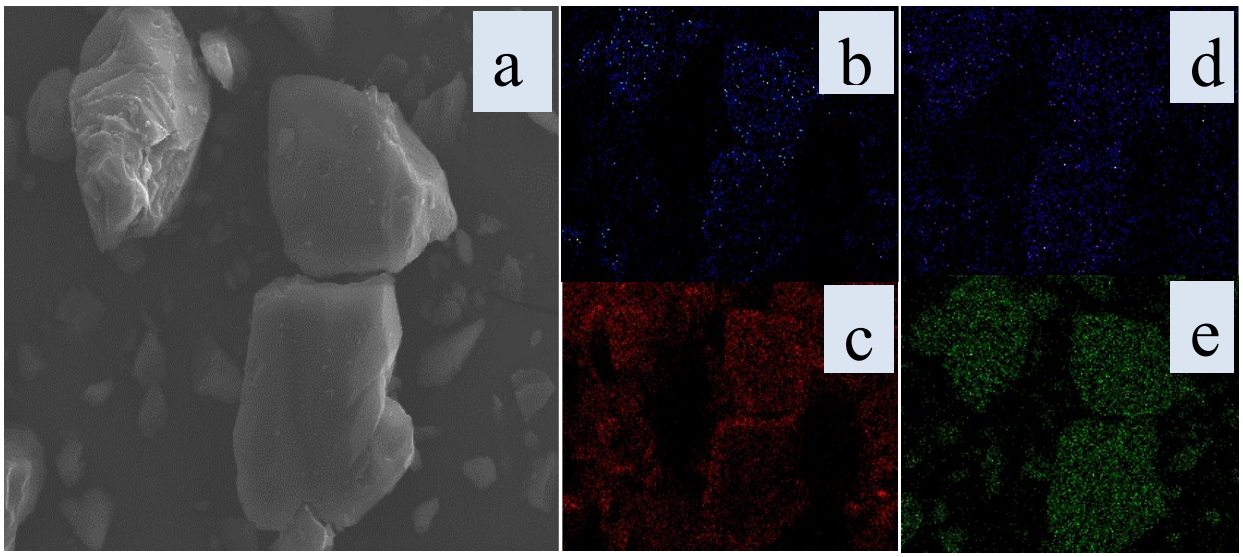


Figure S10. SEM images (a) ZTMOF-1 image (b) N mapping(c) O mapping (d) P mapping (e)Zn mapping.

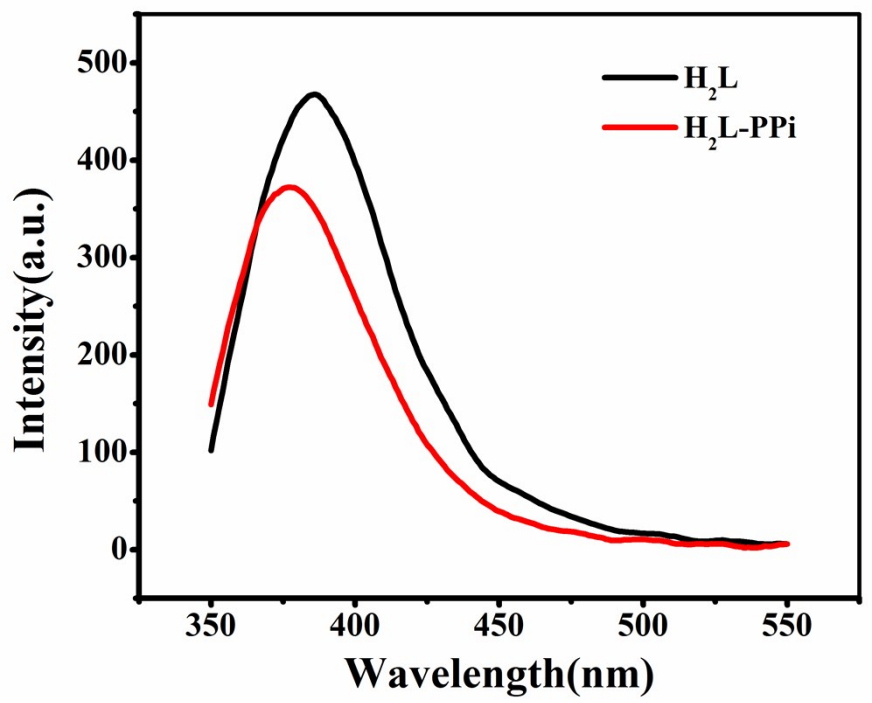


Figure S11. Emission spectra of the H_2L(black line) and H_2L with 400μM PPi(red line).

Table S3. Comparison of different PPi detection methods

Materials	Method	Sensitivity	cyclicity	References
Probe 1+ graphene oxide (GO) complex	Synthesis Probe 1 through three steps of complex chemical reaction then Probe 1 was added to form complexes used for PPi sensing.	2.1μM	unclear	2
carbon dots (CDs)/Pb^{2+} complex	CDs was synthesized by hydrothermal method and then Pb^{2+} was added to form complex which is used for PPi sensing.	54 nM	unclear	3
Eu(DPA)3@ Lap/ Cu2+ complex	$Eu(DPA)_3$@Lap was prepared via ion exchange and coordination and then it was mixed with Cu^{2+} to form complex which is used for PPi sensing.	unclear	unclear	4
N-doped carbon quantum dots (NCQDs)/Fe^{3+} complex	N-CQDs was repared via a simple bottom-up electrochemical (EC) method and then Fe^{3+} was introduced to form complex which is used for PPi sensing.	0.5 μM	unclear	5
MoOx QDs-Fe^{3+} complex	MoOx QDs was prepared via one-step stirring strategy and then Fe^{3+} was introduced to form complex which is used for PPi sensing.	3.3 μM	unclear	6
metal-organic framework(MIL-101(Cr))	luminol-embedded MIL-101 was prepared via solvothermal method，and hydrogen peroxide introduced which could increase the intensity of the MOF gradually, but PPi can inhibit the decomposition of H_2O_2 which is used for PPi sensing.	1.2 μM	unclear	7
ZTMOF-1	ZTMOF-1 was prepared via solvothermal method, and PPi could increase the intensity of the MOF gradually.	2.61μM	At less 5 cycles	**this work**

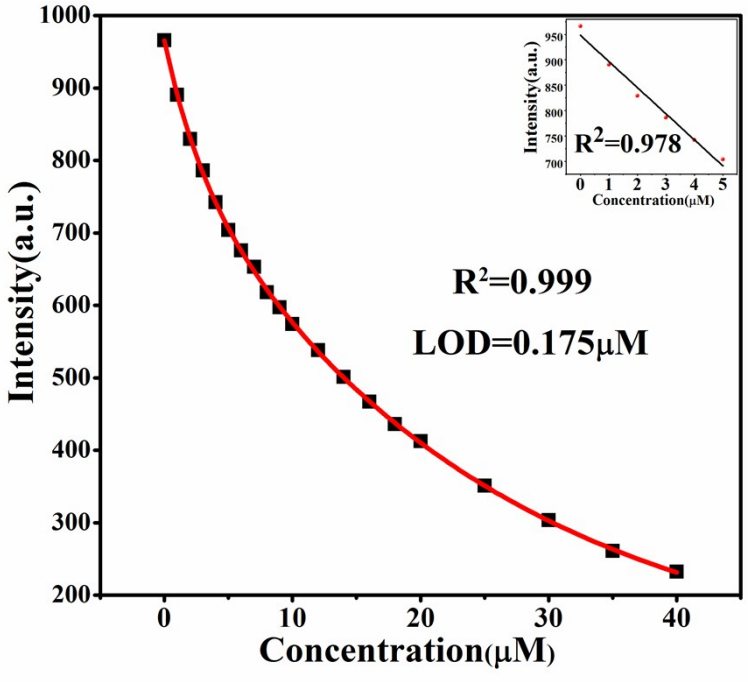


Figure S12. Relationship of the emission intensity of ZTMOF-1and nitrofurantoin concentration from 0-40 μM.

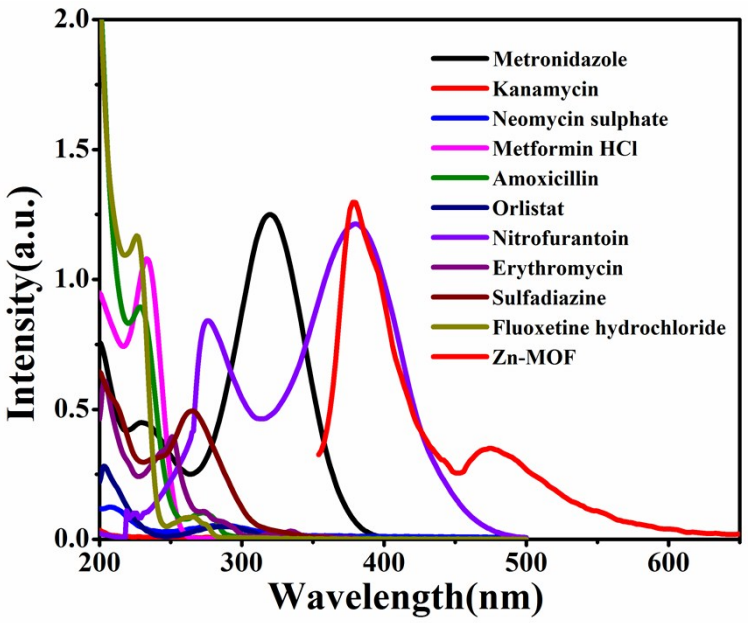


Figure S13. UV-visable spectra of the drugs and emission spectrum of the ZTMOF-1.

References:

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