A luminescent Zn(II) coordination polymer based on a new tetrazolyl-benzimidazolyl tripodal heterotopic ligand for detecting acetone and triethylamine in water

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Supporting Information

Table S1 Crystallographic data and structure refinement summary for Zn-DTPB

Complex	Zn-DTPB
Empirical formula	$C_{18}H_{15}N_{11}OZn$
Formula weight	466.78
Crystal system	Monoclinic
Space group	*P* 21/c
a / Å	9.5220(2)
b / Å	19.44852(5)
c / Å	10.4691(2)
α / °	90
β / °	103.7040(10)
γ / °	90
V / Å^3	1887.12(7)
Z	4
D / g cm^{-3}	1.643
μ / mm^{-1}	2.146
T / K	150(2)
R^a / wR^b	0.0723 / 0.1866
Total / unique	15665 / 3865

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S2 Selected bond lengths [Å] and angles [°] for Zn-DTPB

Zn-DTPB			
Zn(1)-N(3)[1]	2.014(2)	Zn(1)-N(1)	1.981(3)
Zn(1)-N(5)[2]	1.993(2)	Zn(1)-N(9)[3]	1.995(3)
N(1)-Zn(1)-N(3)[1]	106.57(11)	N(1)-Zn(1)-N(5)[2]	120.04(11)
N(1)-Zn(1)-N(9)[3]	106.97(10)	N(5)[2]-Zn(1)-N(3)[1]	110.46(10)
N(5)[2]-Zn(1)-N(9)[3]	108.05(10)	N(9)[3]-Zn(1)-N(3)[1]	103.49(10)

Symmetry transformations used to generate equivalent atoms: [1]-1 + x, y, Z; [2]-1 + x, 1/2 - y, 1/2 + z; [3]-x, 1 - y,1 - z.

Table S3 Comparisons of the acetone sensing performances of Zn-DTPB and reported MOFs.

MOFs	Detection medium	fluorescence quenching efficiencies (65%)	fluorescence quenching efficiencies (85%)	References
Zn-DTPB	H_2O	0.52%	1.47%	This work
$[Cd_2(btec)(TPB)_{0.5}(H_2O)_4]\cdot 2H_2O$	H_2O	1.9%	4.5%	*Inorg. Chem. Front.*, 2021, **8**, 3096–3104
$[Zn_6(1,4\text{-bpeb})_4(IPA)_6(H_2O)]_n$	H_2O	0.75%	1.59%	*Molecules*, 2023, **28**, 7315.
$Tb(BTC)(H_2O)_6$	H_2O	1.11%	2.79%	*J. Mater. Chem.*, 2012, **22**, 6819-6823
Eu(BTC) (MOF-76)	1-propanol	0.58%	1.18%	*Adv. Mater.*, 2007, **19**, 1693-1696
$[Tb_4(\mu_6\text{-}L)_2(\mu\text{-}HCOO)(\mu_3\text{-}OH)_3(\mu_3\text{-}O)(DMF)_2(H_2O)_4]_n\cdot(H_2O)_{4n}$	DMF	21%	60%	*ACS Appl. Mater. Interfaces.*, 2018, **10**, 23976-23986
$[Cd_3(tib)_2(BTB)_2]\cdot 3DEF\cdot 4.5H_2O$	CH_3CN	0.81%	1.44%	*Inorg. Chem.*, 2016, **55**, 11821-11830
$[Cd_3(tib)_2(BTB)_2(DMA)_2(H_2O)_2]\cdot 2DMA\cdot 8H_2O$	CH_3CN	0.86%	1.50%	*Inorg. Chem.*, 2016, **55**, 11821-11830
$Yb(BPT)(H_2O)(DMF)_{1.5}(H_2O)_{1.25}$	1-propanol	0.75%	3.85%	*Chem. Commun.*, 2011, **47**, 5551-5553
$\{[Cd_3(L)(H_2O)_2(DMF)_2]\cdot 5DMF\}_n$	1-propanol	2.79%	5.40%	*J. Mater. Chem.*, 2012, **22**, 23201-23209
$\{[Cd_3(L)(dib)]\cdot{}_3H_2O\cdot 5DMA\}_n$	1-propanol	2.83%	4.89%	*J. Mater. Chem.*, 2012, **22**, 23201-23209
$[Cu(dmpy)_3(H_2O)_2](H_2O)(ClO_4)_2$*	Acetonitrile	0.0002%	0.0004%	*RSC Adv.*, 2020, **10**, 42137-42146

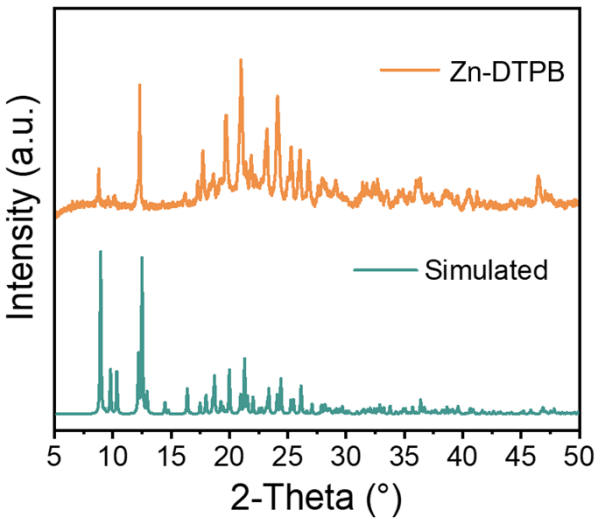

Fig. S1 PXRD of simulated and as-synthesized Zn-DTPB.

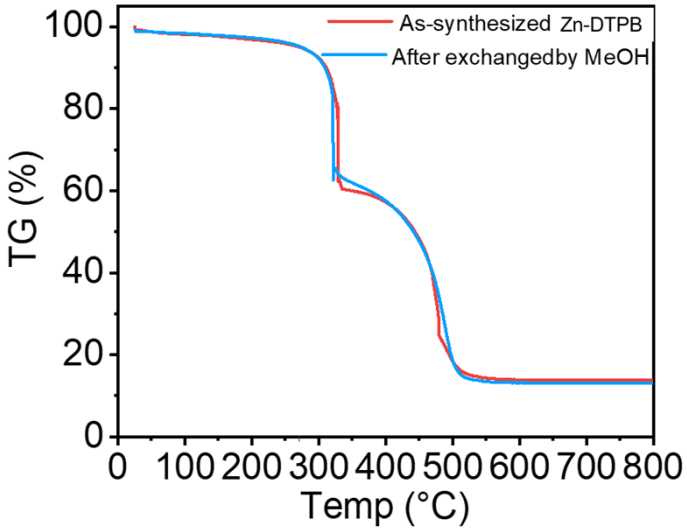

Fig. S2 TG curve of Zn-DTPB before and after immersing in water.

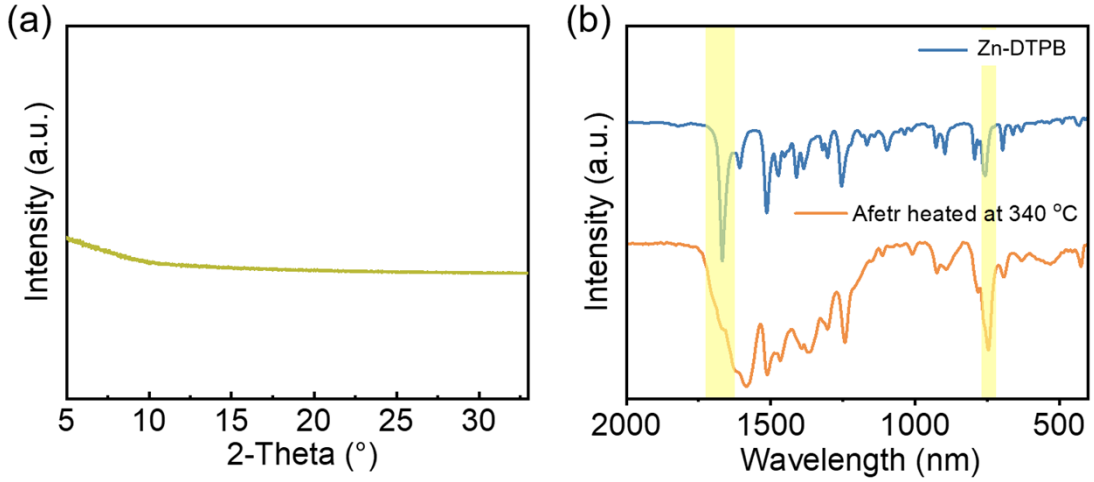

Fig. S3 (a) PXRD of Zn-DTPB after heated at 340 °C. (b) IR of Zn-DTPB before and after heated at 340 °C.

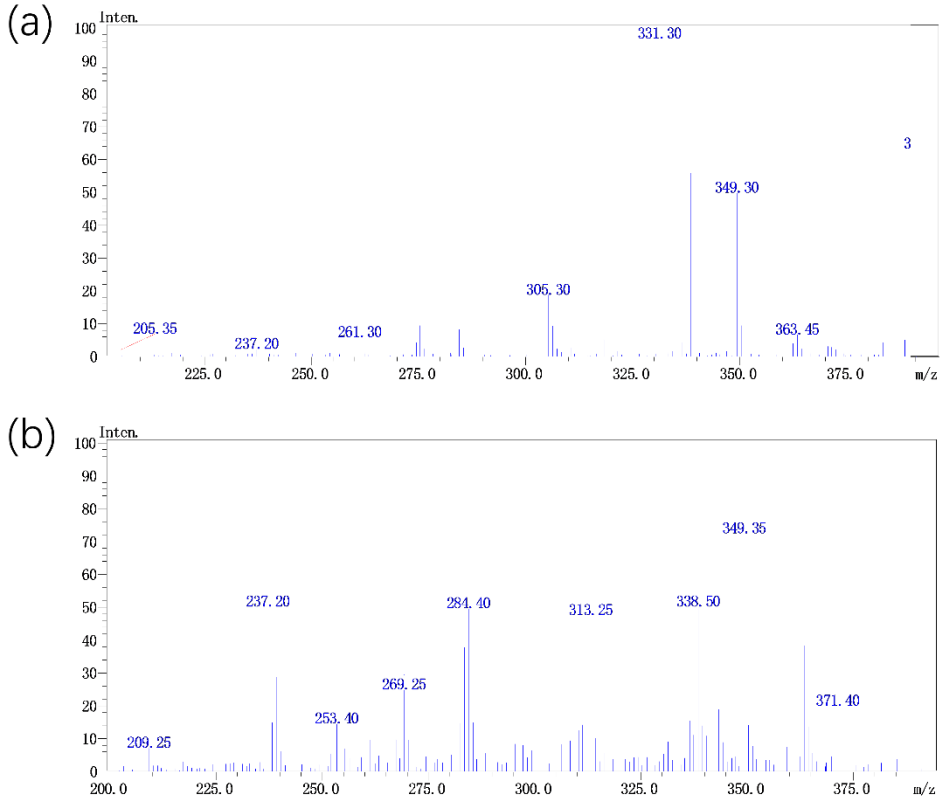

Fig. S4 MS spectra of (a) as-synthesized Zn-DTPB and (b) Zn-DTPB after heating at 340 °C that were digested by HCl.

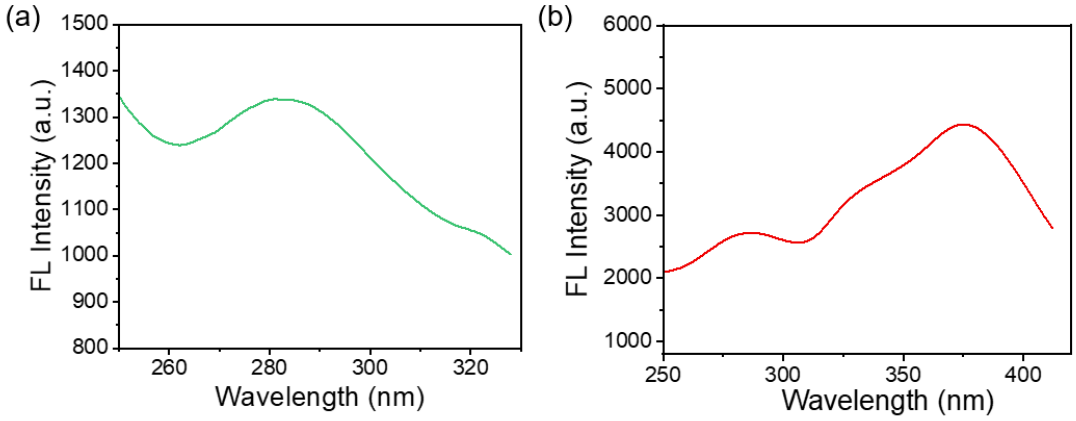

Fig. S5 Excitation spectra of (a) H_2DBPT and (b) Zn-DTPB.

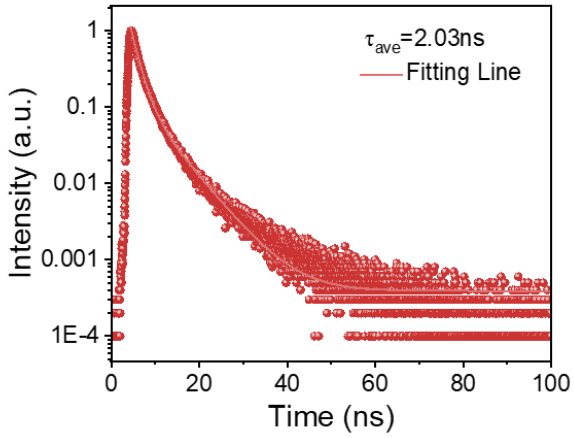

Fig. S6 Time-resolved fluorescence spectra of Zn-DTPB.

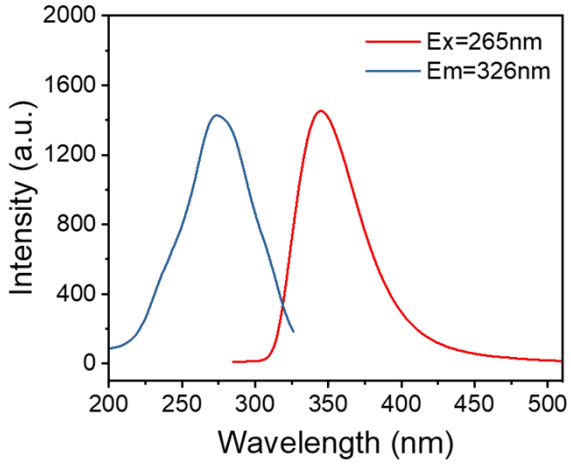

Fig. S7 Fluorescent excitation and emission spectra of Zn-DTPB after dispersed in water.

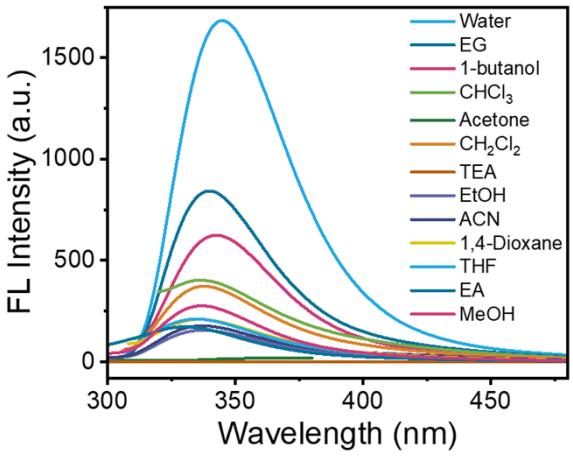

Fig. S8 Fluorescent spectra of Zn-DTPB after dispersed in various solvents.

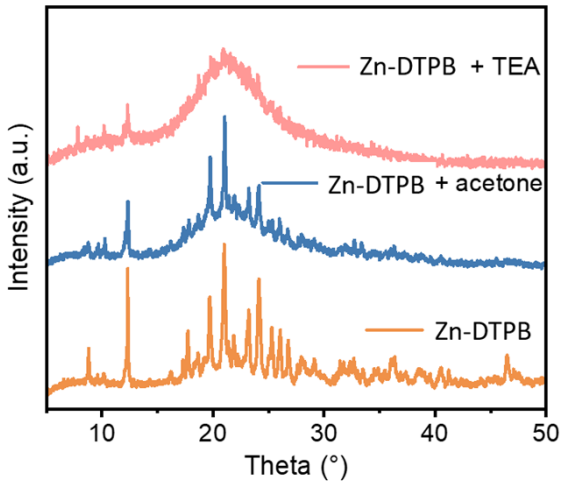

Fig. S9 The PXRD patterns of Zn-DTPB before and after sensing acetone and TEA.

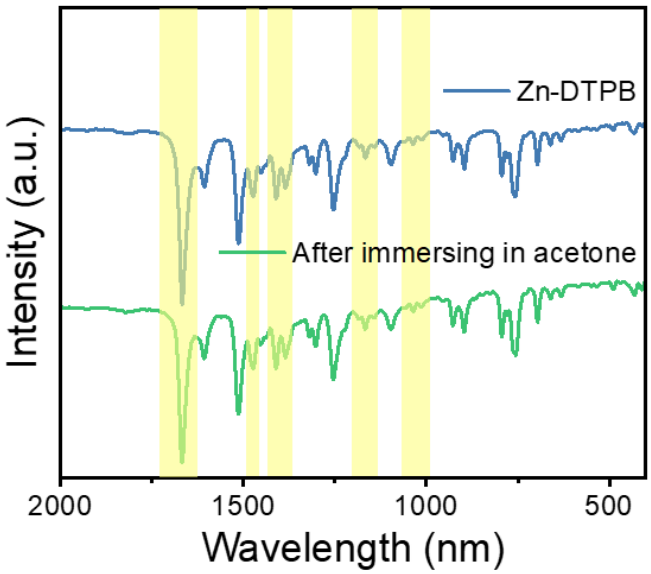

Fig. S10 The IR spectra of Zn-DTPB before and after immersing in acetone.

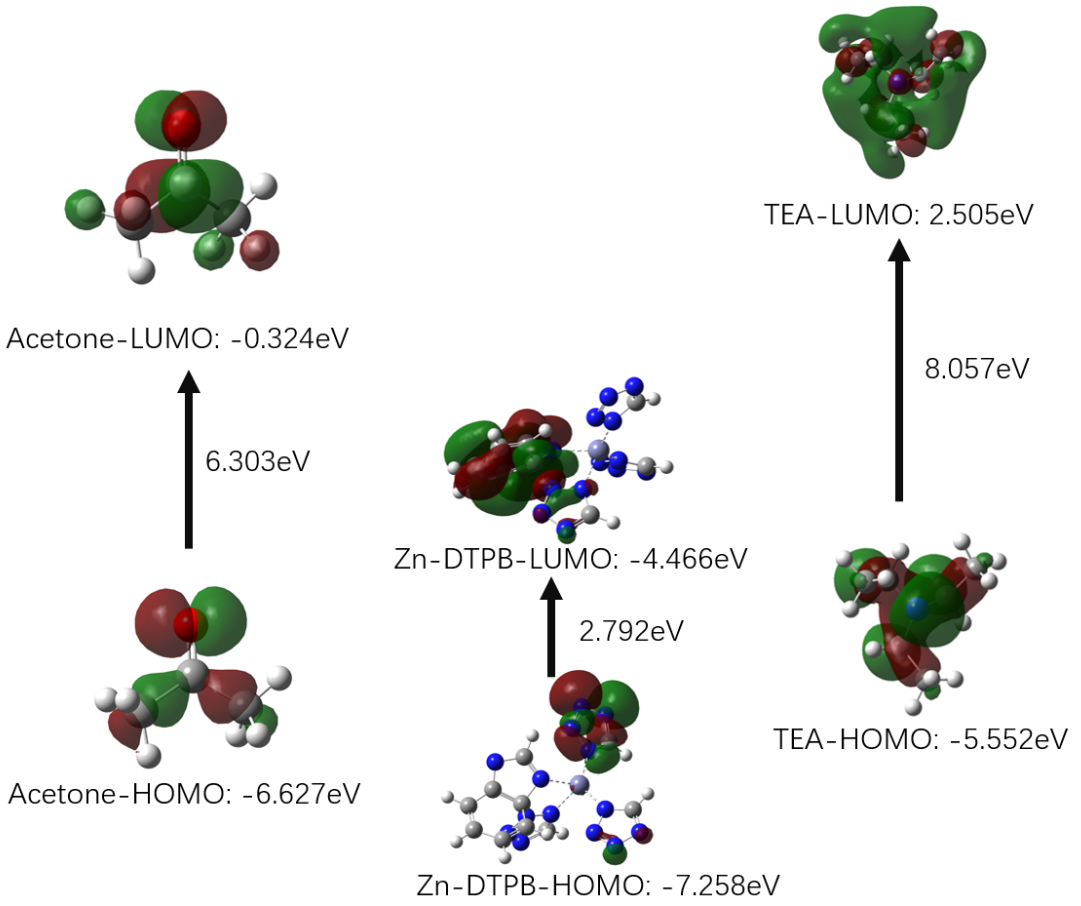

Fig. S11 HOMO and LUMO energy level diagram for the acetone, Zn-DTPB, and TEA.

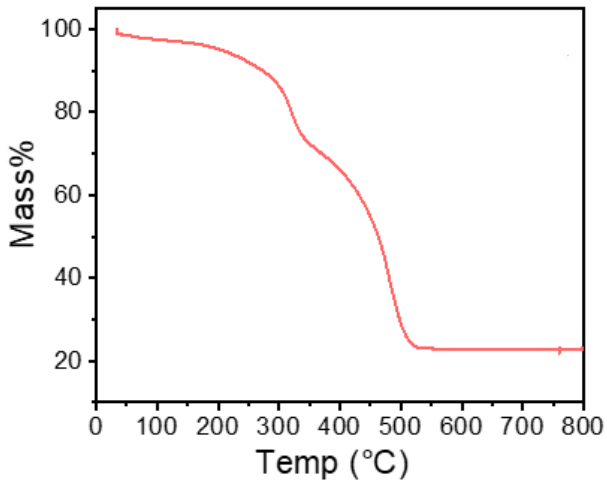

Fig. S12 The TG curve of *a*Zn-DTPB.

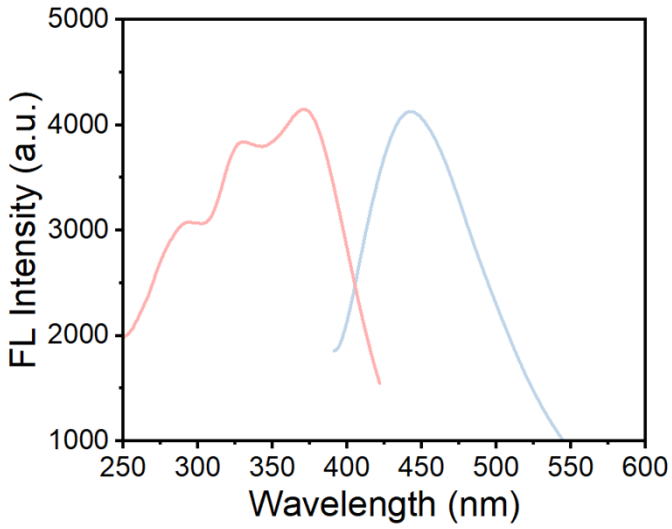

Fig. S13 Solid-state fluorescent excitation and emission spectra of aZn-DTPB.

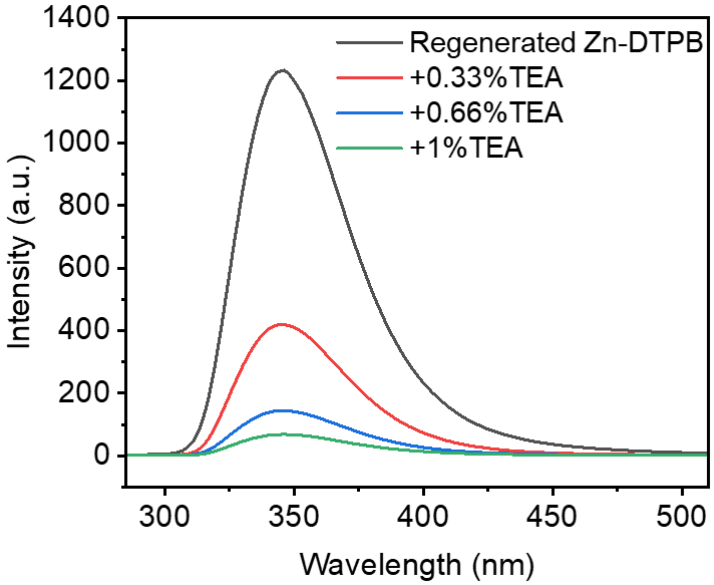

Fig. S14 Fluorescence spectra of a suspension of Zn-DTPB regenerated from aZn-DTPB with the addition of 0% to 1% (Vol%) TEA.