Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Zn-MOF Constructed from Electron-rich π-conjugated Ligand with Interpenetrated Graphene-like Net as Efficient Nitroaromatic Sensor

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Table S1. Crystal structure refinement details of Zn-MOF.

Formula	$C_{30}H_{23}N_3O_5Zn$
Formula weight	571.73
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	9.861 (2)
b (Å)	28.306 (6)
c (Å)	10.024 (2)
β (°)	102.863(4)
Volume (Å^3)	2727.9(10)
Z	4
Density (calculated)	1.388
M (Mo K*α*)(mm^{-1})	0.94
F(000)	1176
Theta range for data collection	2.2°-25°
R_{int}	0.048
Observed data [$I > 2\sigma(I)$]	3675
R_1, wR_2 (all data)	0.0613, 0.1348
S	1.03
Min. and max resd dens (eÅ^{-3})	0.52 −0.35

[a]$R_1 = \Sigma||Fo| - |Fc||/|Fo|$; $wR_2 = [\Sigma w(\Sigma F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Coordinates of 4-(bis(4-(pyridin-4-yl)phenyl)amino)benzoic acid used in DFT calculation.

Atom Type	x	y	z
C	15.67808412697428	73.46076370377210	25.11606033432005
C	16.15769179869603	72.09728862345030	22.67470556198033
C	16.31574432683411	69.47197057942542	22.63671984266031
C	16.93705426477145	68.21173233335315	20.45851200136376
C	17.45481254764571	69.53241494351971	18.23765113658217
C	17.29130993220013	72.14168581123637	18.27309286501875
C	16.61731581695695	73.40085424555474	20.44060005465375
C	30.68035744293621	73.04032768449672	9.26581482144204
C	28.81824432300364	71.93039798984481	10.69688310734790
C	26.33482126324401	72.70547660553186	10.46649123953544
C	25.87338054921393	74.64665003294959	8.77610182981825
C	27.83904532609929	75.67955328132206	7.42367753528361
C	24.25107126325252	71.51049687644637	11.91217956735184
C	24.58897666875869	70.75307015469836	14.40931985425552
C	22.61967850033500	69.66721122450876	15.73415991669912
C	20.28885788329568	69.32380165151284	14.60324363424004
C	19.96548604394284	70.01276042101244	12.11604442169224
C	21.91480055890570	71.11894577452578	10.80902747749242
C	12.16822798220169	54.78024576337255	14.54060522063585
C	12.84403879132431	57.23760336203805	15.03790907202839
C	14.56808303657962	58.46681706724775	13.46220263950943
C	15.40739646303756	57.11457501034170	11.38575439386628
C	14.62076721388547	54.68770704666181	11.00657486023395
C	15.47279750883784	61.04452848822491	14.03794014441712
C	13.93042283671979	62.80276410572894	15.24634917063590
C	14.80607017667133	65.17507166996089	15.86850367631138
C	17.28949323643096	65.87793799226094	15.33550817264332
C	18.83731799585652	64.13360992755737	14.10691199780593
C	17.92715343629080	61.77734953963365	13.45664856624245
N	30.23345029316973	74.92105674782017	7.65355989891770
N	13.04750871369157	53.47561032951421	12.57247461193958
N	18.23417501561086	68.24436159184654	16.01577479156251
O	15.09855818983806	75.77048728040198	25.04760396231334
O	15.88518743899014	72.30269248019552	27.13919586274066

H	15.92671736800348	68.34339596621193	24.43002212142881
H	17.03491006041638	66.05968616288719	20.44972479377980
H	17.71829429469452	73.27202296633746	16.48956322742687
H	16.43671476867008	75.54693870615185	20.38902057722551
H	32.68179016600992	72.28049769976980	9.50639981717066
H	29.31804564589159	70.36016086503777	12.08451047113762
H	23.86811198635238	75.38641755507737	8.50666221282408
H	27.46221295892586	77.26893246817045	6.01910398443787
H	26.49774699443652	71.02814742565630	15.36946777754172
H	22.90863186771232	69.04600735500910	17.77660144468187
H	18.07735566038098	69.66509227649453	11.13877976356725
H	21.57291241008219	71.71922439672831	8.76850456387794
H	10.78411707369769	53.86009097389498	15.91119190350440
H	11.99818680853896	58.26567358671296	16.73159196068691
H	16.76264175773913	58.02749186530161	9.98188520441856
H	15.30710358209553	53.58946997949595	9.28501352613426
H	11.89704606417643	62.29160512442838	15.74137552788205
H	13.49572837273815	66.58892570927017	16.83026081855602
H	20.87424288037764	64.64866732692639	13.63087776984065
H	19.23947344332614	60.41992649431002	12.41926022487739
H	16.78581681469492	76.92863950897863	25.50776784131309

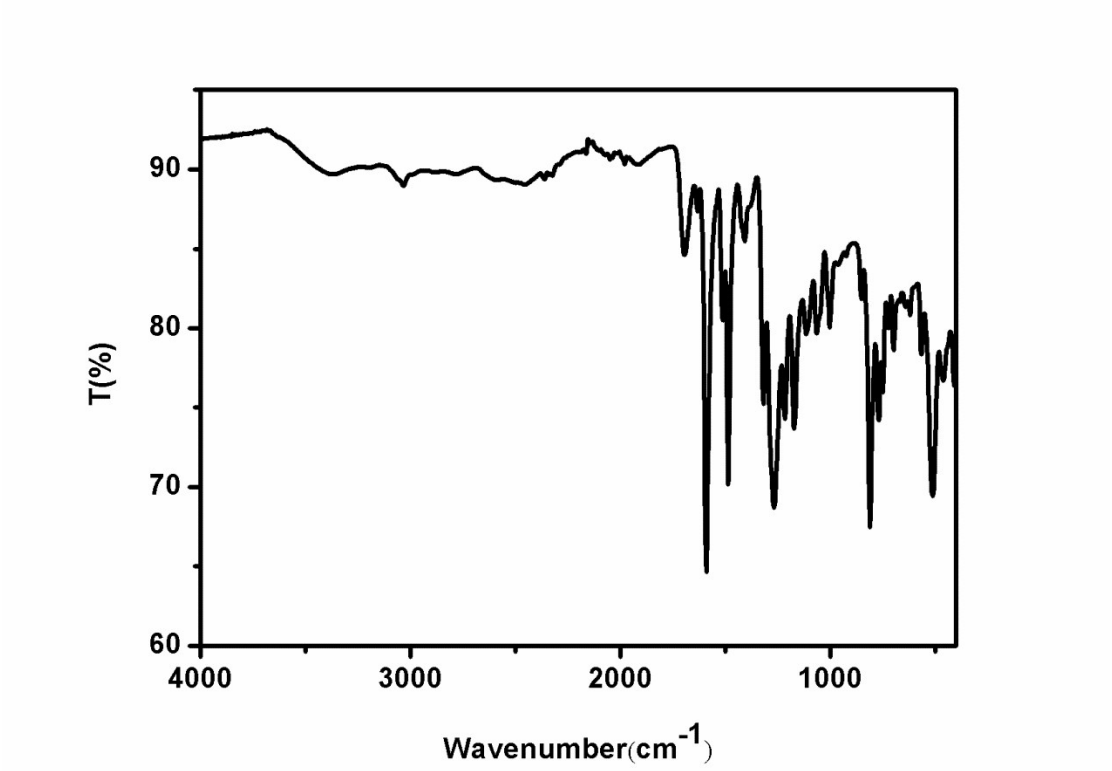

Figure S1. IR spectrum of ligand (HL).

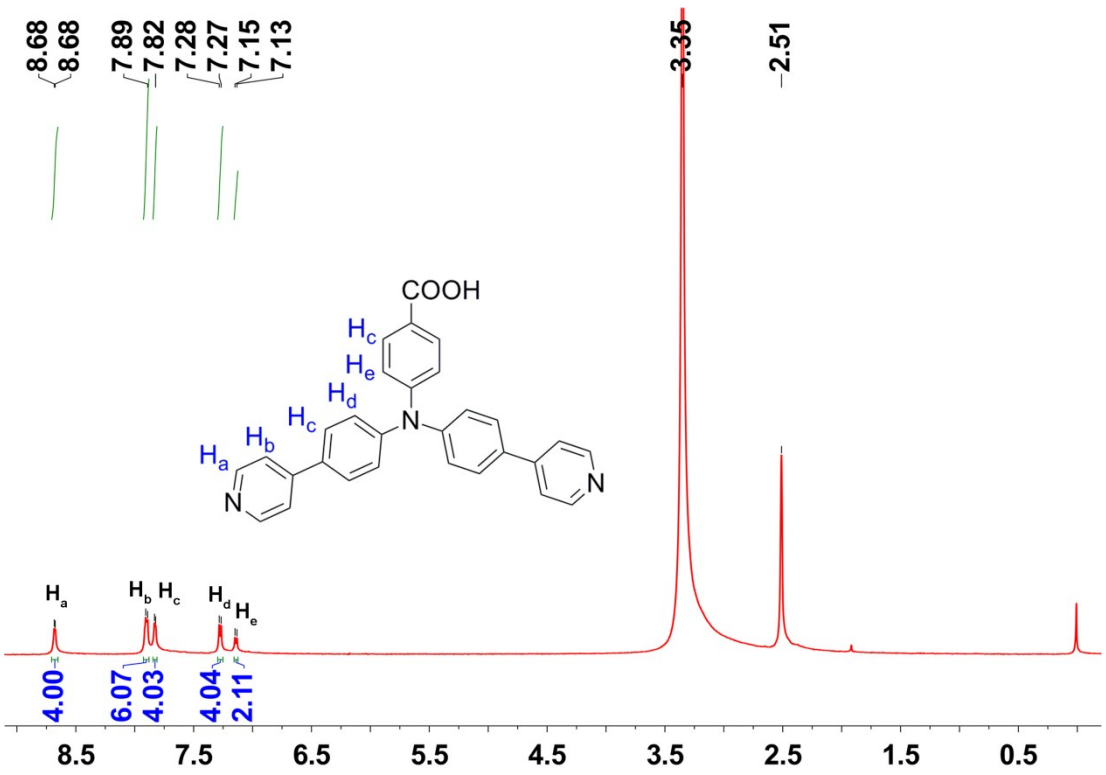

Figure S2. ^{1}H NMR of Ligand (HL).

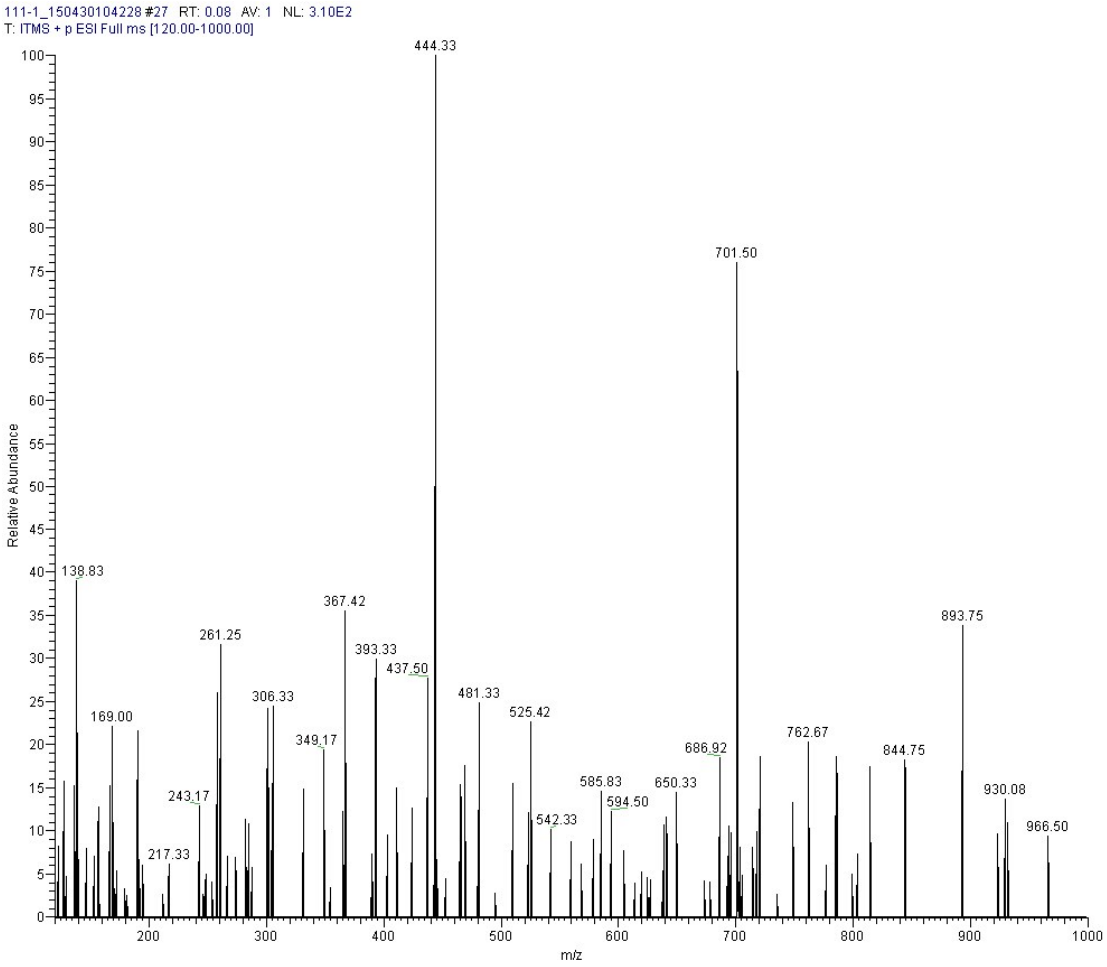

Figure S3. Mass Spectrum of Ligand (HL).

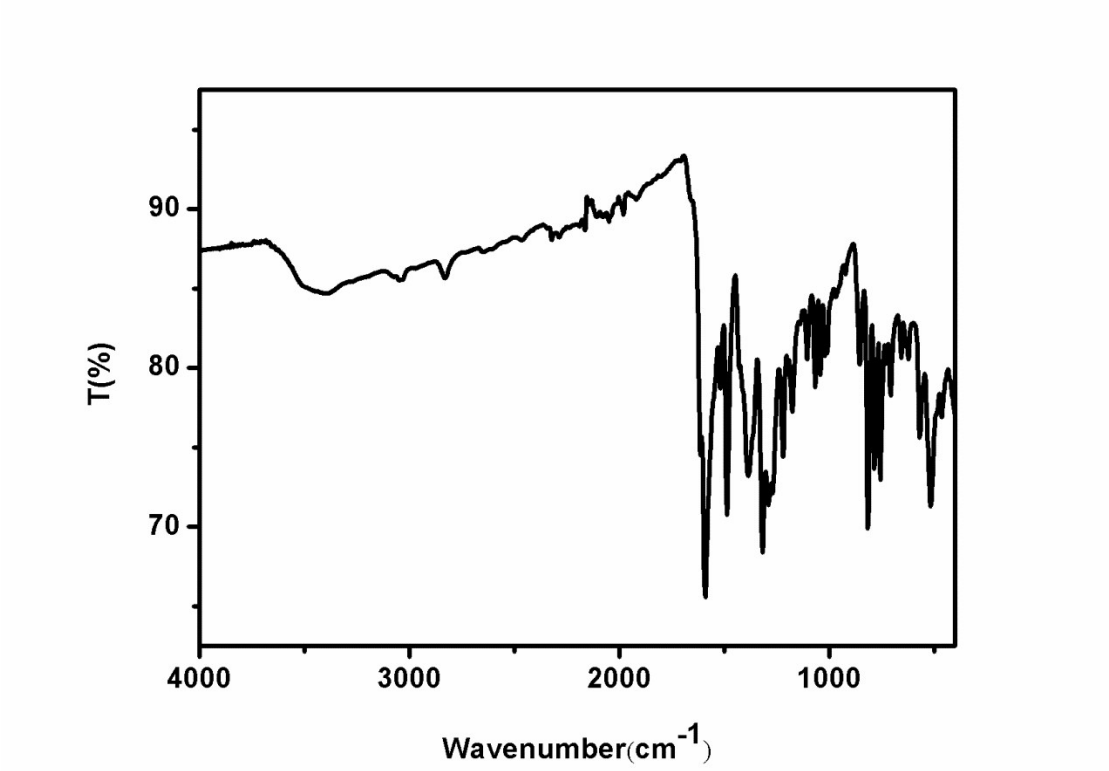

Figure S4. IR spectrum of Zn-MOF.

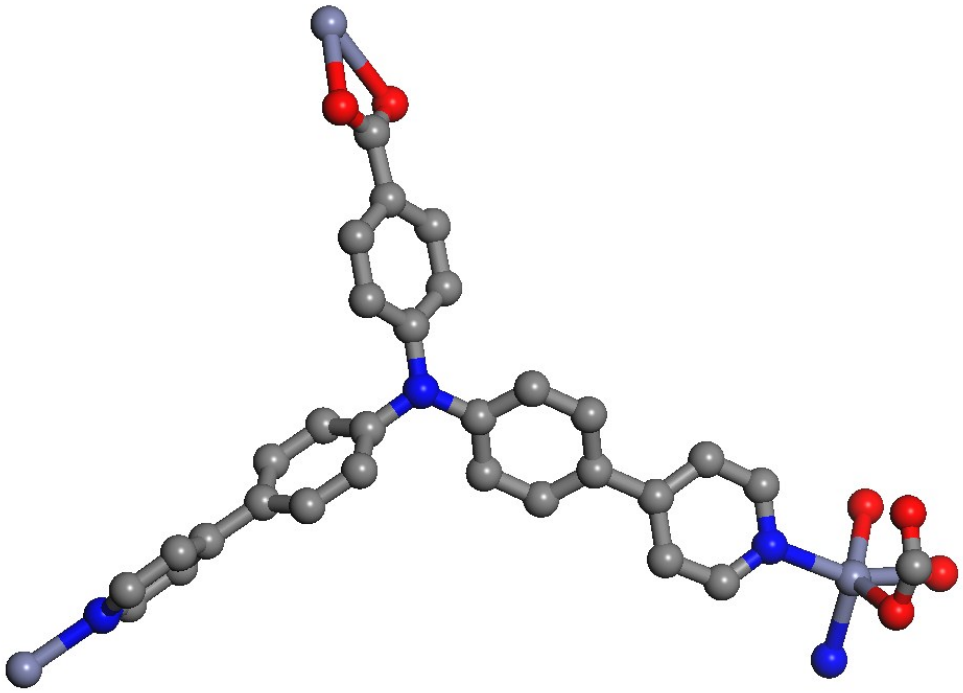

Figure S5. Asymmetric unit of Zn-MOF.

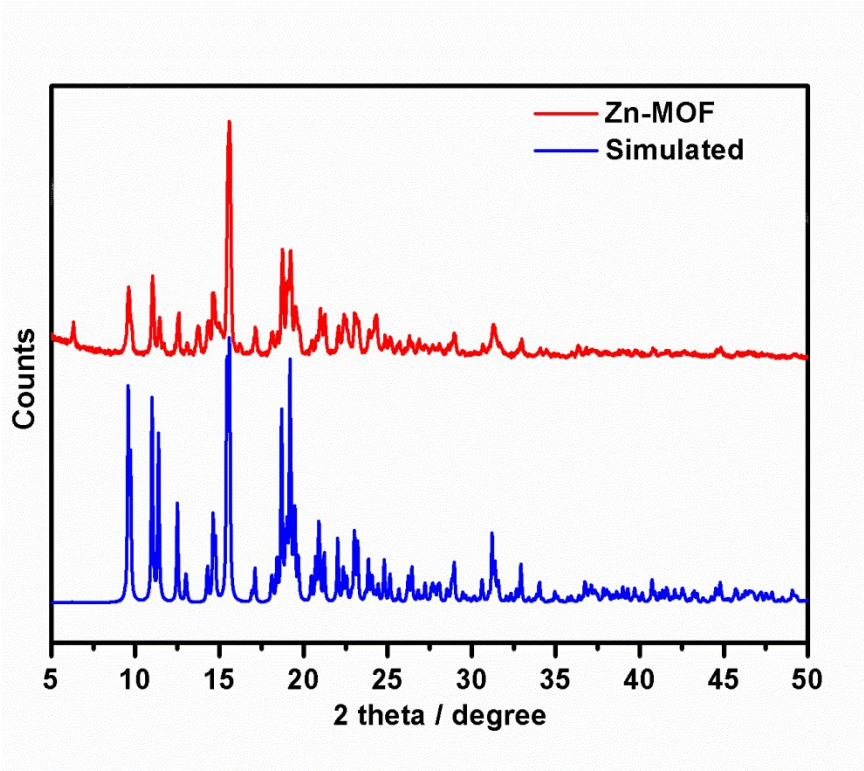

Figure S6. **PXRD patterns of** Zn-MOF. Collected from as-synthesized sample (red) and the simulated one (blue) based of single crystal X-ray diffraction data.

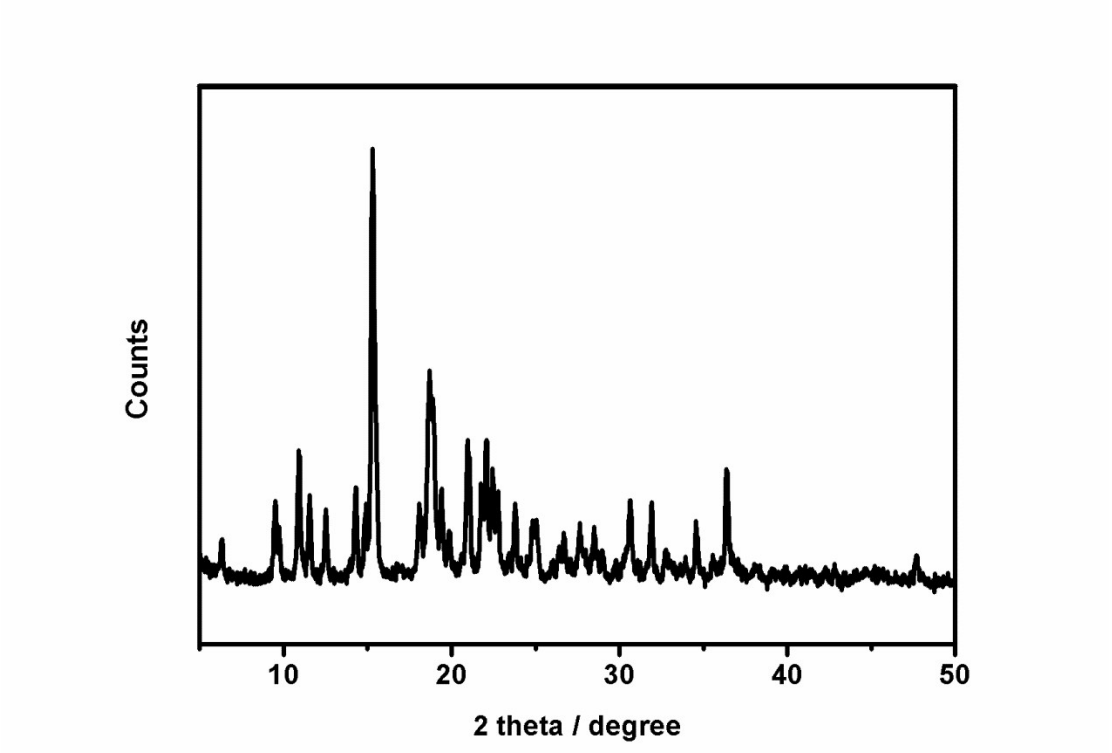

Figure S7. PXRD pattern of Zn-MOF after 3 days in H_2O.

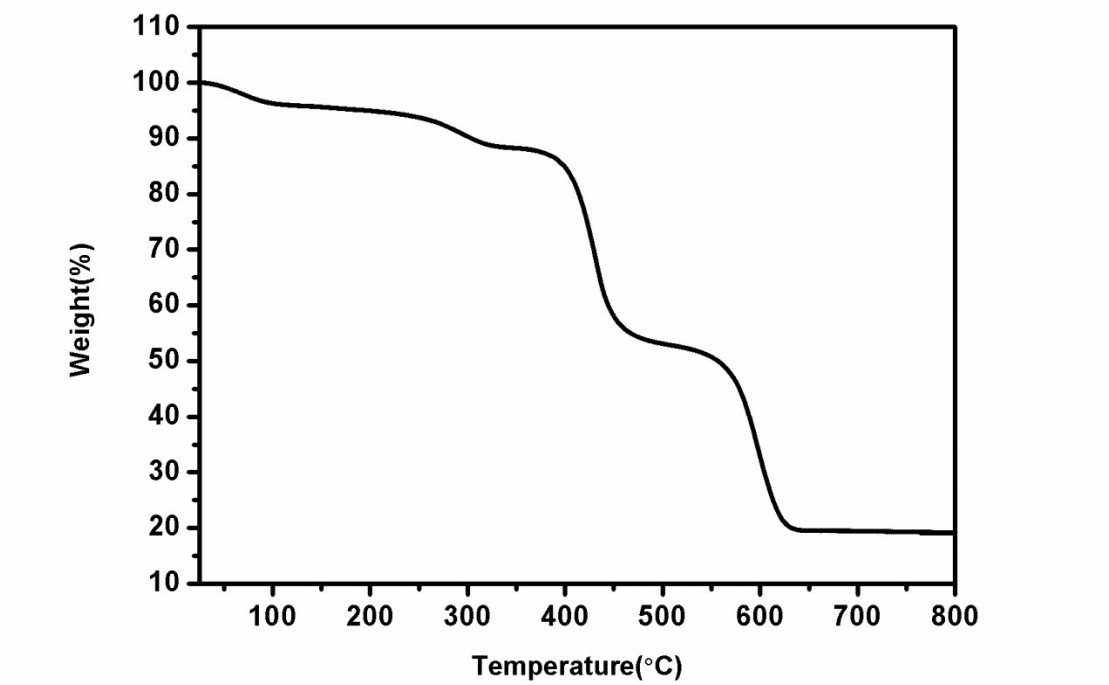

Figure S8. TGA curve of Zn-MOF.

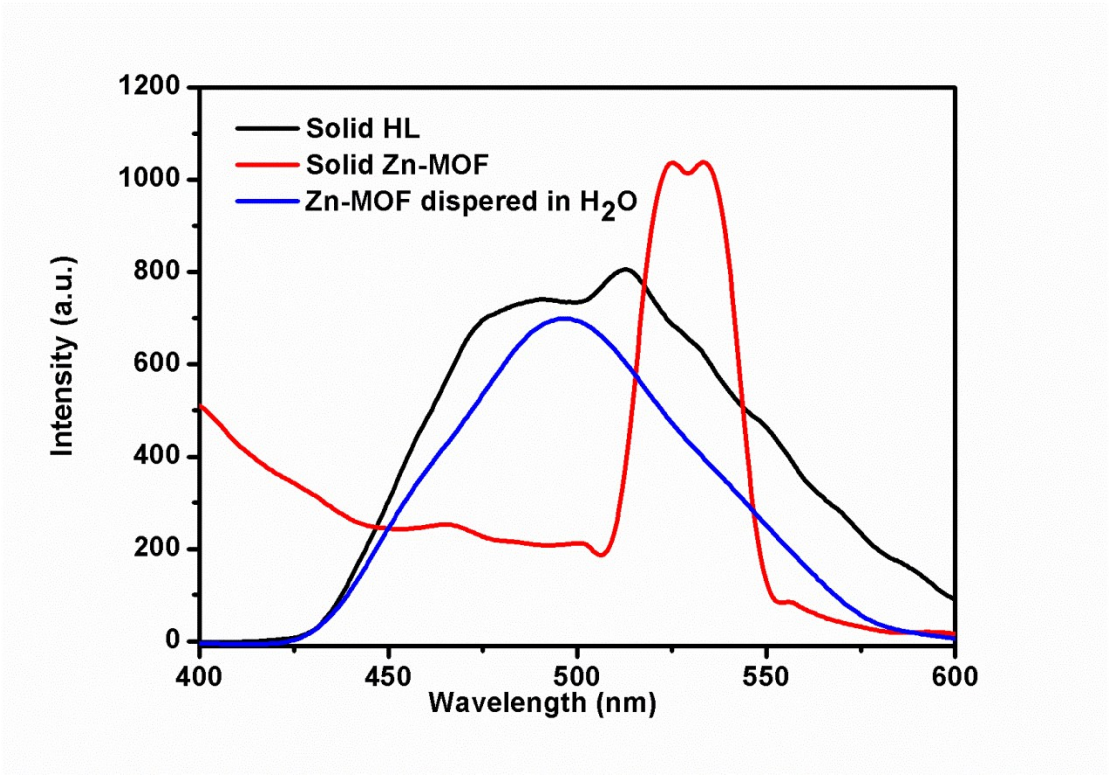

Figure S9. Emission spectra of HL ligand (λ_{ex} =395 nm) and Zn-MOF **(λ_{ex} =401 nm) in solid state, as well as Zn-MOF dispersed in water.**

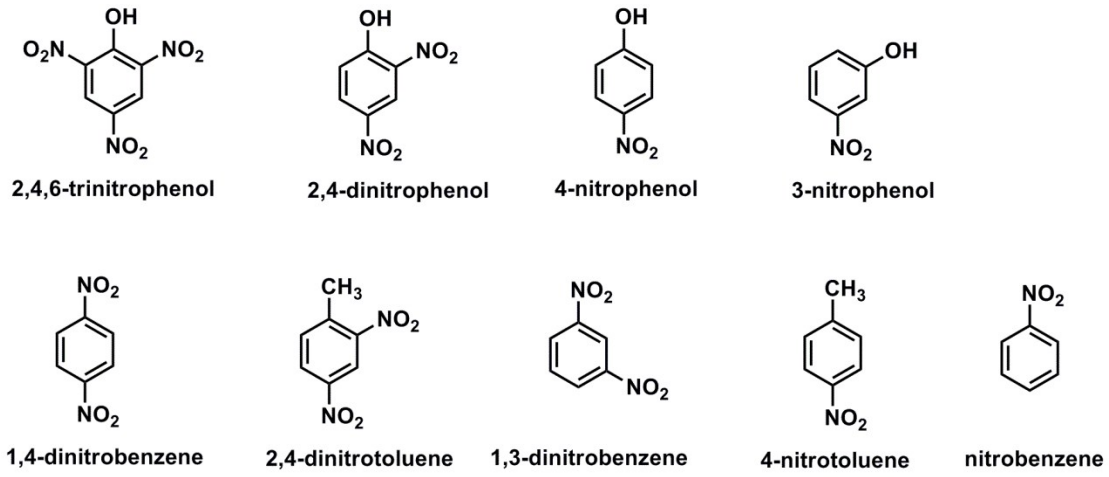

Figure S10. Chemical structures of the analysts used in the sensing experiments.

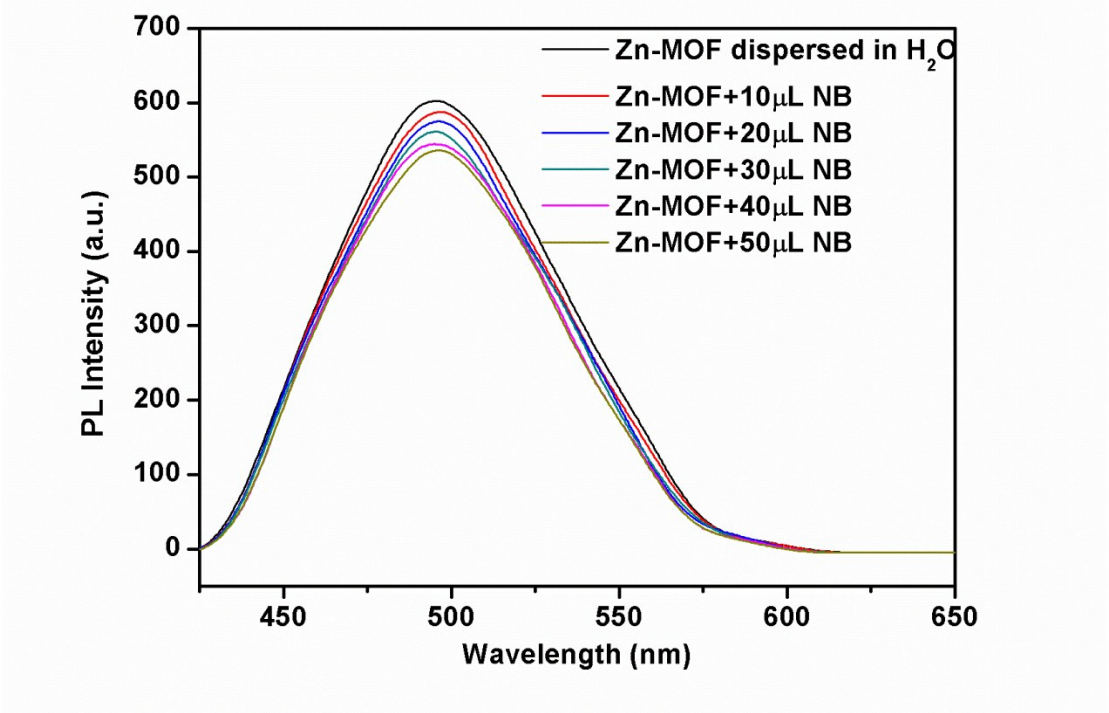

Figure S11. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of nitrobenzene (NB).

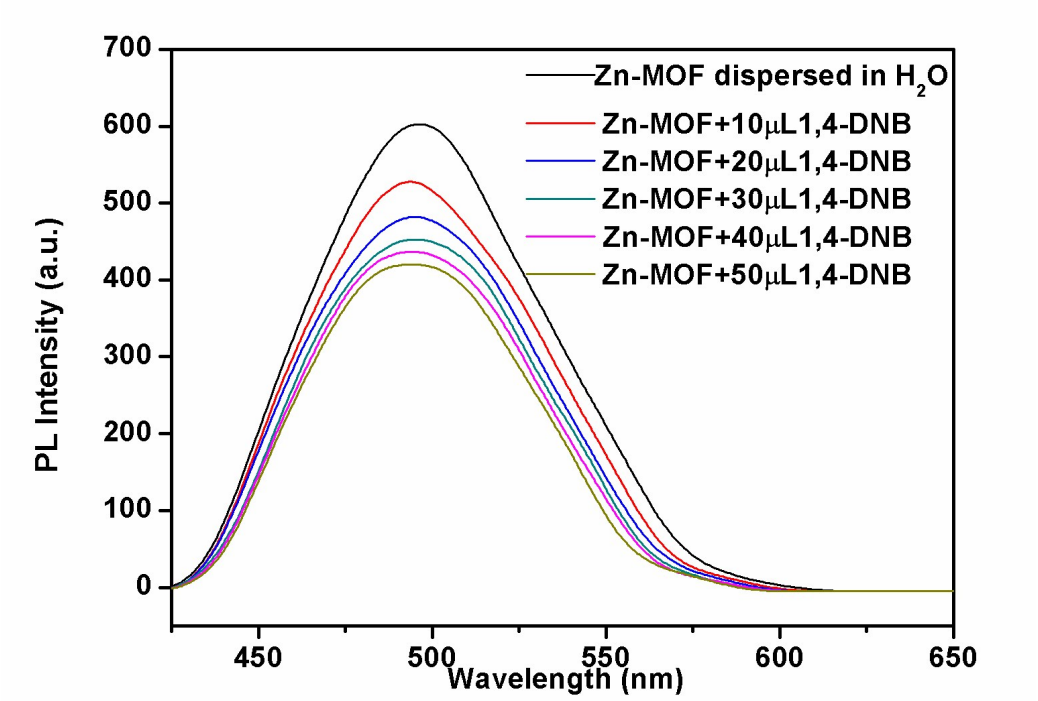

Figure S12. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 1,4-dinitrobenzene (1,4-DNB).

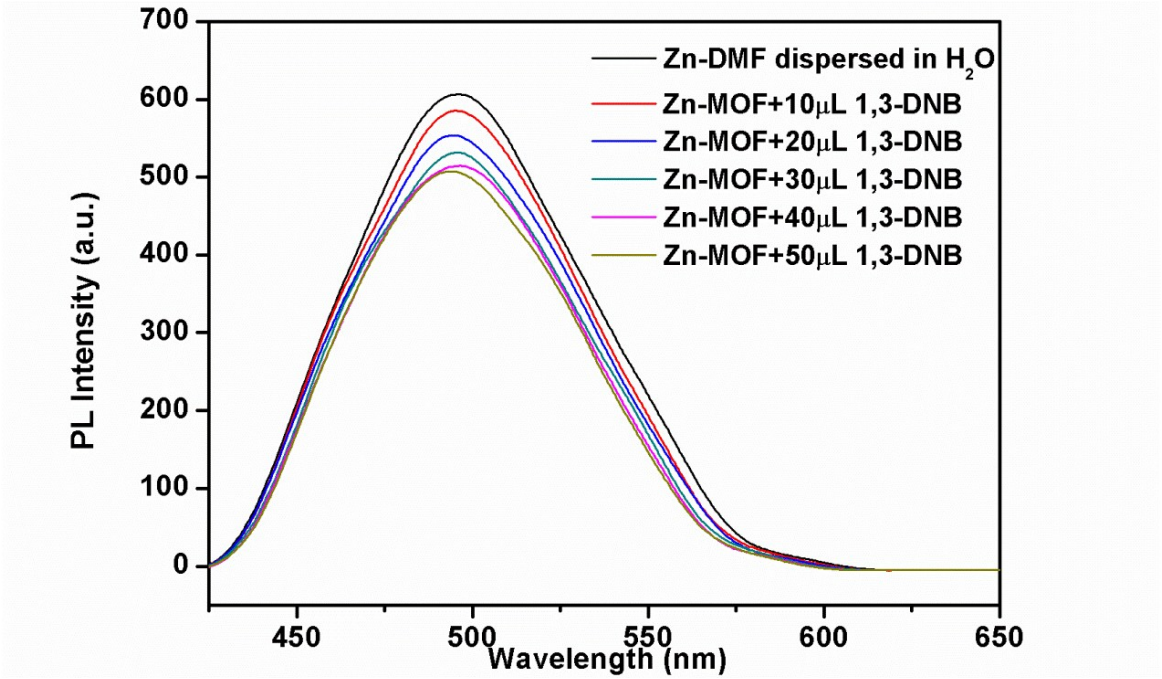

Figure S13. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 1,3-dinitrobenzene (1,3-DNB).

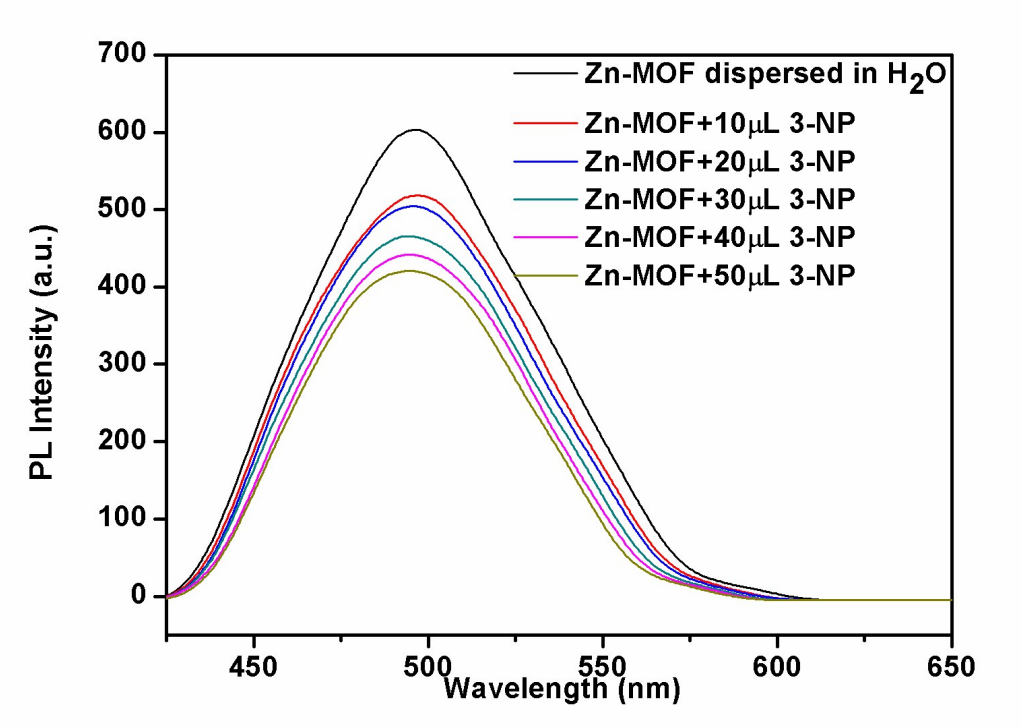

Figure S14. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 3-nitrophenol (3-NP).

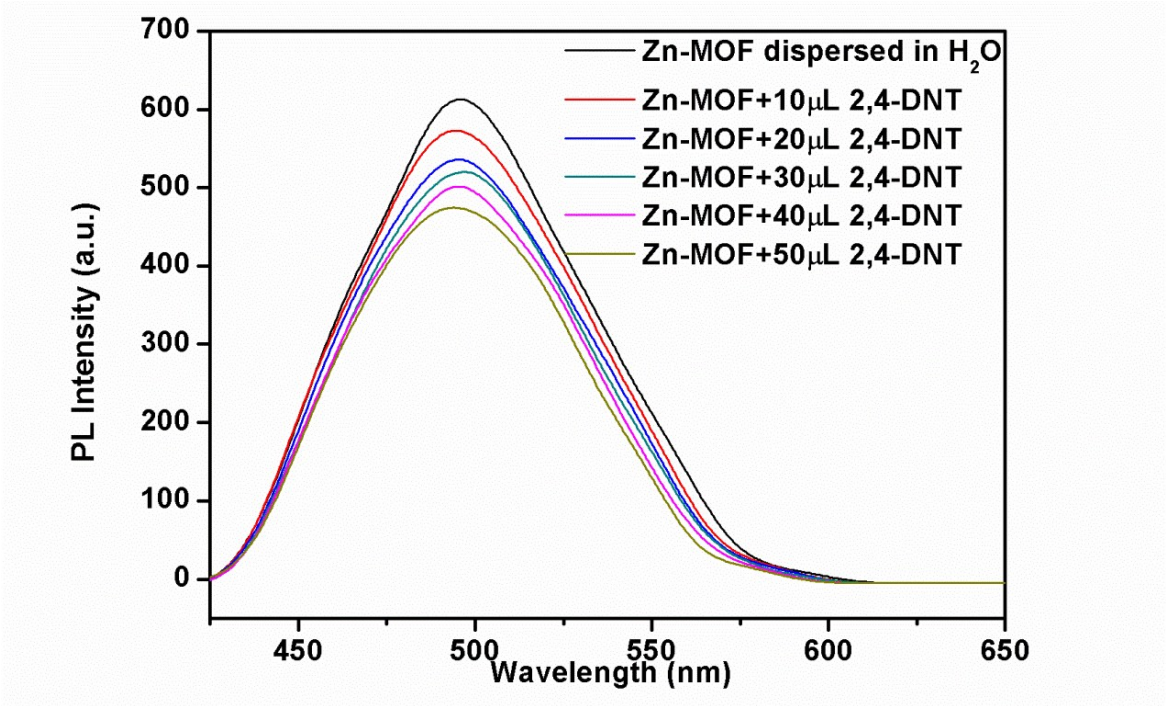

Figure S15. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 2,4-dinitrotoluene (2,4-DNT).

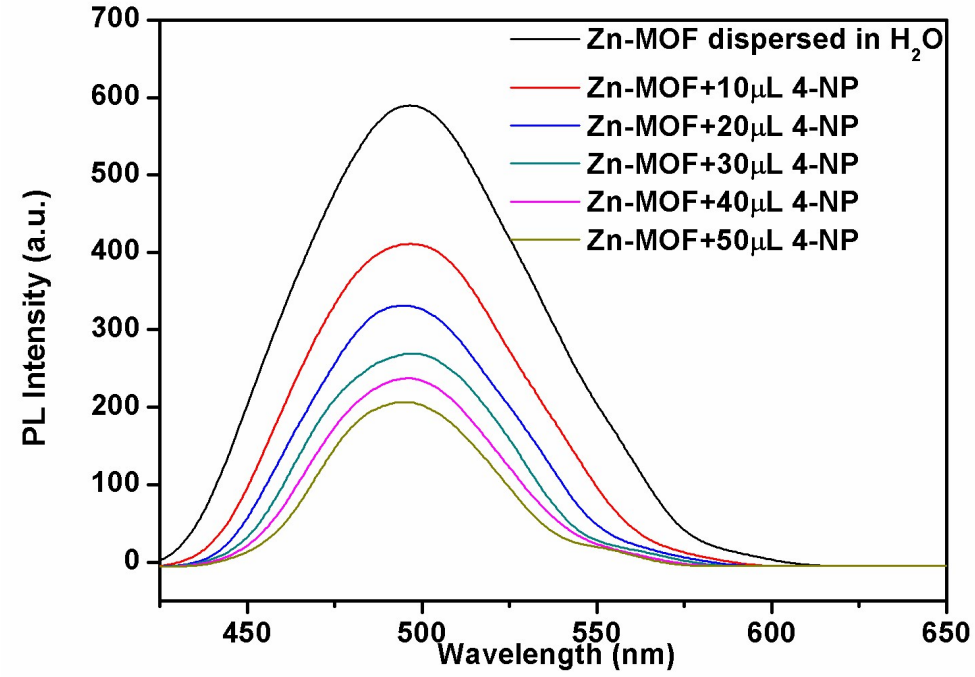

Figure S16. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 4-nitrophenol (4-NP).

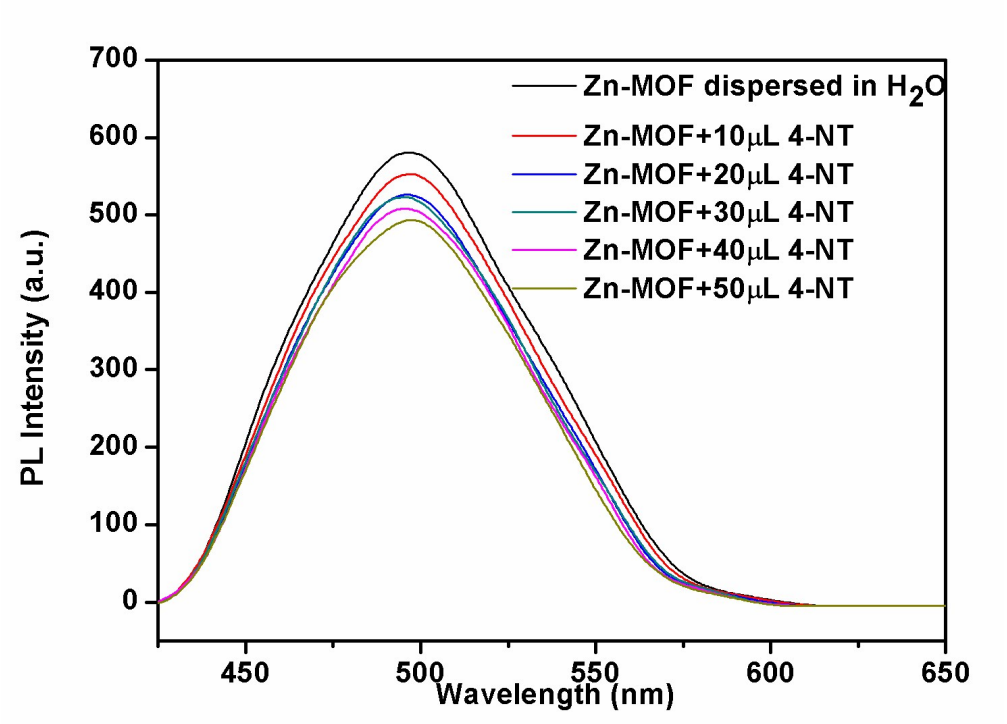

Figure S17. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 4-nitrotoluene (4-NT).

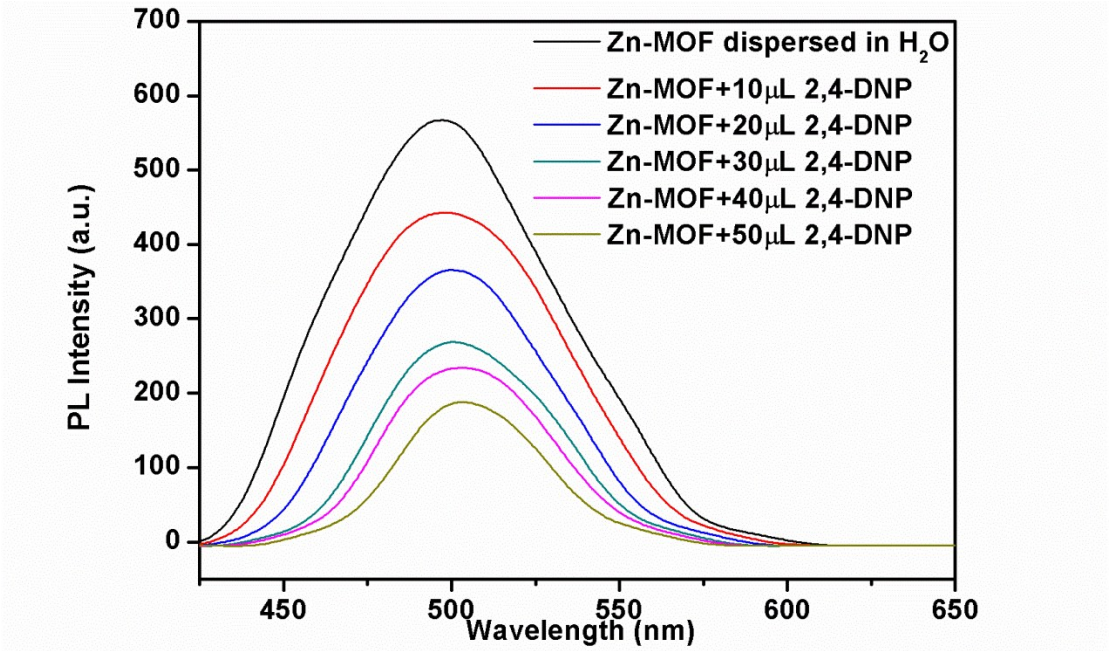

Figure S18. Fluorescent titrations of 0.5 mg Zn-MOF dispersed in in 2 mL H_2O solution with the addition of different volume of 5 mM solution of 2,4-dinitrophenol (2,4-DNP).

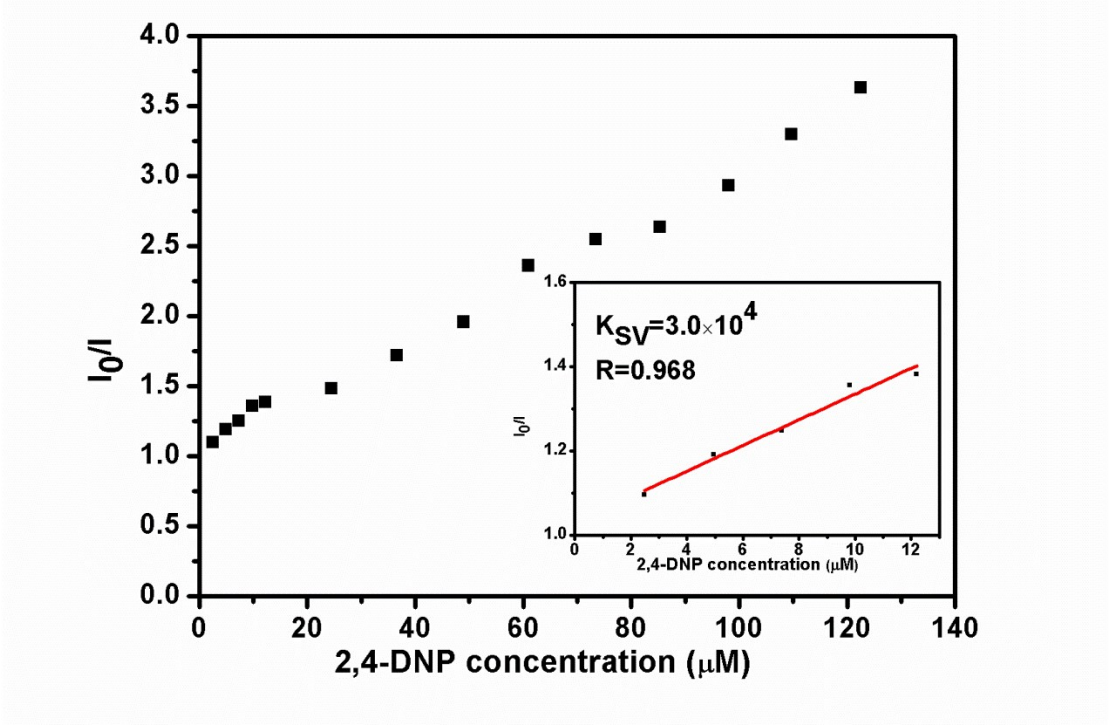

Figure S19. Stern–Volmer plot of I_0/I versus 2,4-DNP concentration in the Zn-MOF H_2O suspension (insert: enlarged view of a selected area).

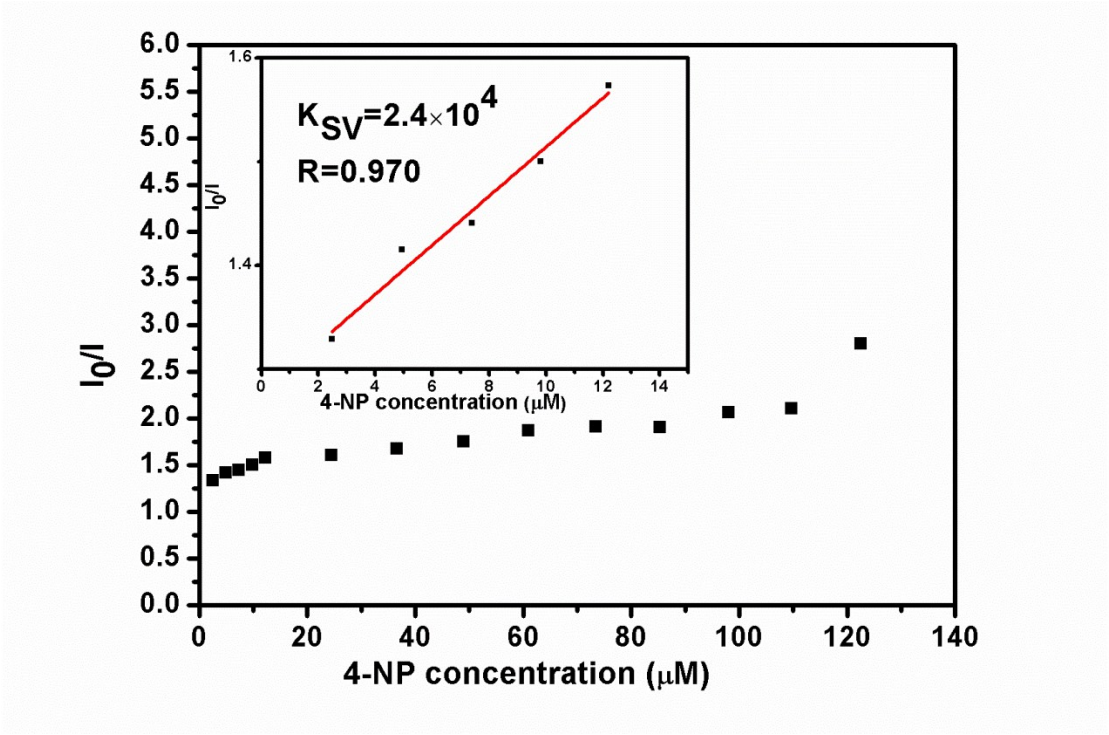

Figure S20. Stern–Volmer plot of I_0/I versus 4-NP concentration in the Zn-MOF H_2O suspension (insert: enlarged view of a selected area).

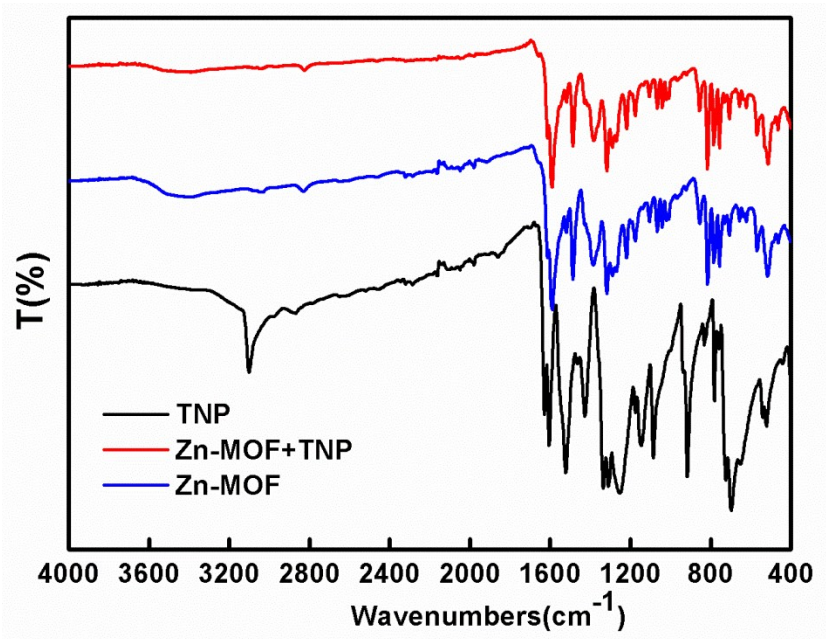

Figure S21. IR spectra of TNP, as-synthesized Zn-MOF, and Zn-MOF after immersing in TNP solution for 1 h.

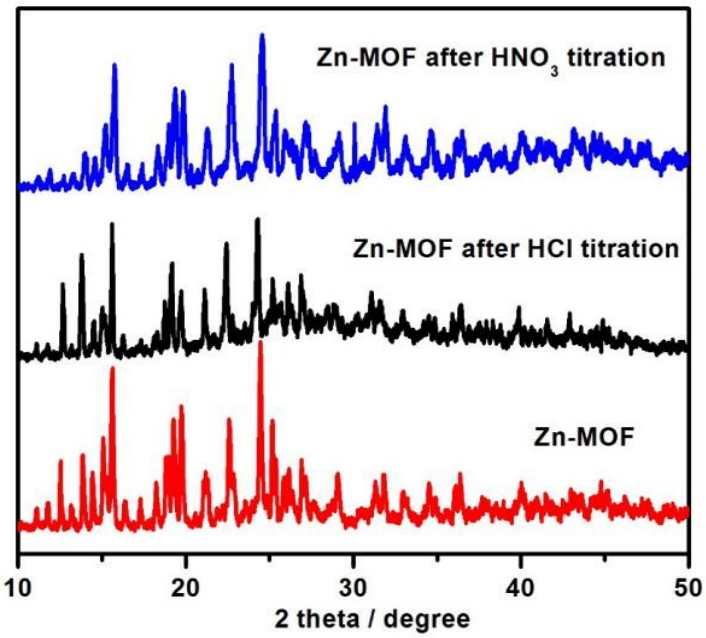

Figure S22. PXRD patterns after titration with HCl and HNO_3.

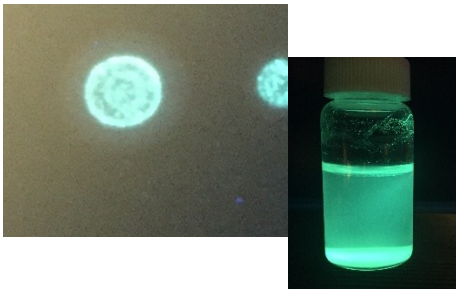

Figure 23. UV irradiated image of solid state Zn-MOF(left) and the suspended MOF(right).