Supporting information

Materials and General Methods.

All chemicals and solvents of reagent grade were commercially purchased and used for synthesis without any further purification. Elemental analysis (C, H, N) was measured using a German Elementary Vario ELIII instrument. Powder X-ray diffraction (PXRD) patterns were collected by a Rigaku MiniFlex 600 diffractometer using Cu Kα radiation (λ=1.5406Å). Thermogravimetric analyses (TGA) were measured on an NETZSCH STA 449 C instrument with a heating rate of 10 °C min^{-1} under a flowing nitrogen atmosphere. Fluorescence spectrum in the liquid state were recorded on a Horiba Jobin-Yvon Fluorolog-3 spectrofluorometer. In situ FT-IR spectra were recorded using a NICOLET 6700 instrument at 298 K. The solid and solution state UV-Vis spectra of compounds and analytes were obtained by a Cary 5000 UV-Vis spectrometer from Agilent Technologies using a quartz cuvette of path length 10 mm.

Single-Crystal X-ray Data Collection and Refinements.

The single-crystal data of **FJI-H26** was collected on a Mercury CCD diffractometer with graphite monochromated Mo Kα radiation (λ=0.71073 Å) at 293K. The structure was solved by SHELXL package and all the non-hydrogen atoms were refined anisotropically. In theory, the hydrogen atoms of organic ligands are formed on a specific atom and refined iso-tropically. Crystal data and structure refinement parameters of the crystal are summarized in Table S1. The CCDC number is 1994306 and these data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Synthesis of FJI-H26

A mixture of $ZnCl_2$ (0.04mmol, 5mg) and H_2DTBDA (0.02mmol, 7.5mg) in 5 mL DMA/MeOH (v_1:v_2=1:1) was sealed in a 23 mL Teflon vial, heating this solution at 85℃ for 3 days led to the colourless crystal of **FJI-H26** with 70% yield. IR (KBr, cm^{-1}): 3145, 2949, 2877, 2358, 2337, 1614, 1525, 1365, 1280, 1207, 1145, 1124, 1039,

979, 891, 842, 796, 727, 659, 594, 567, 493. Anal. calcd for $[Zn(DTBDA)](DMA)(MeOH)_2(H_2O)_{3.5}$: C, 44.08; H, 5.24; N, 14.99. Found: C, 44.00; H, 5.20; N, 15.24.

Typical fluorescence quenching experiment

10mg crystal of **FJI-H26** and 15ml DMF were put in a glass bottle, the suspension of **FJI-H26** could be obtained through ultrasonic treatment for 2 hours. Transfering 2ml of **FJI-H26** suspension into a dry and clean fluorescent cuvette, then different analytes were added into such suspension, and corresponding fluorescence could be obtained immediately.

Recycling experiment

A 2ml suspension of **FJI-H26** in DMF or benzyl alchol solution was put into the cuvette, and the initial fluorescence was firstly recorded. After that, 10μL *p*-NA or 50μL benzaldehyde was added into the suspension, and the corresponding fluorescence was tested. The used **FJI-H26** samples could be isolated through centrifugation and filtration. The fluorescence of used **FJI-H26** samples could be restored after three times of DMF solution washing.

Anti-interference experiment

A 2ml suspension of **FJI-H26** was put into the cuvette, and the initial fluorescence was firstly recorded. After that, 10μL interfering nitroaromatic solution (0.01M) was added to the suspension, and the fluorescence driven by interfering nitroaromatic was recorded. Finally, 10μL *p*-NA solution (0.01M) was added to such mixed suspension, and the anti-interference fluorescence could be obtained.

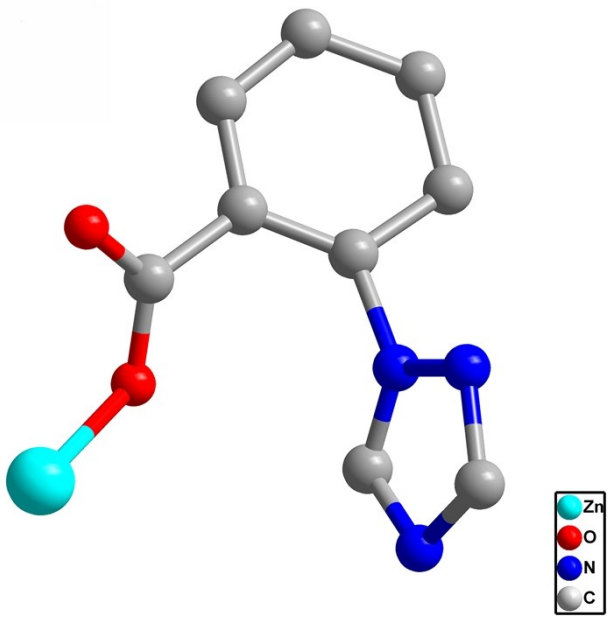

Figure S1. The asymmetric unit of **FJI-H26**. (For clarity, All hydrogen atoms and solvent molecules are omitted.)

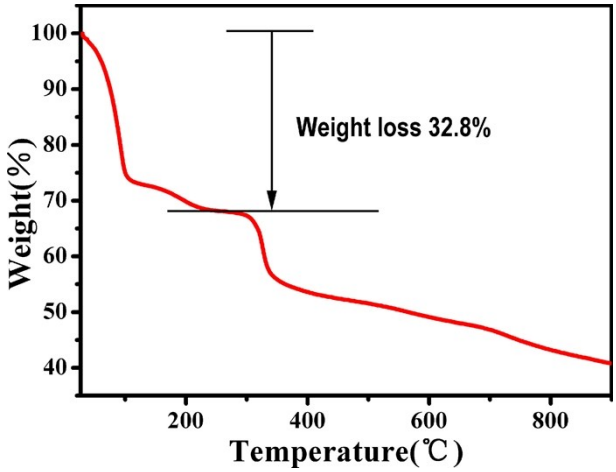

Figure S2. TGA curve of as prepared **FJI-H26.**

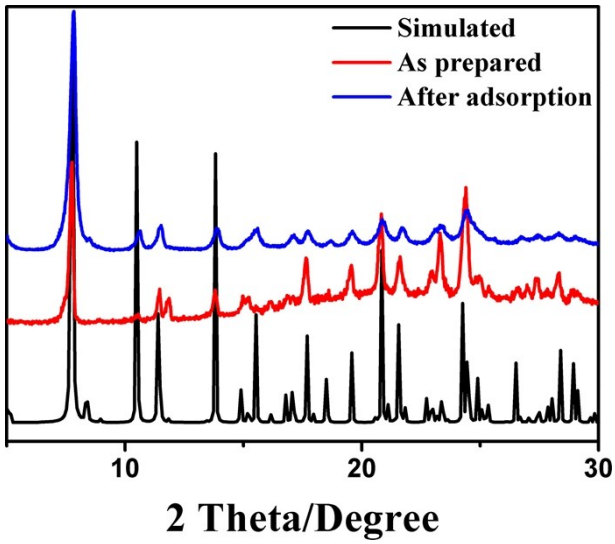

Figure S3. PXRD patterns of fresh prepared and after gas sorption sample of **FJI-H26**.

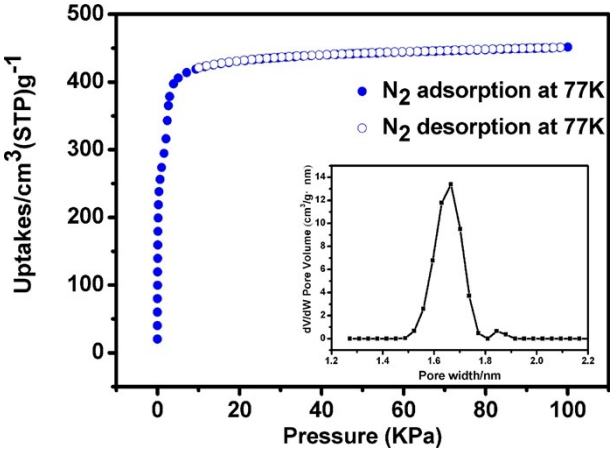

Figure S4 N_2 sorption isotherms for **FJI-H26** at 77K

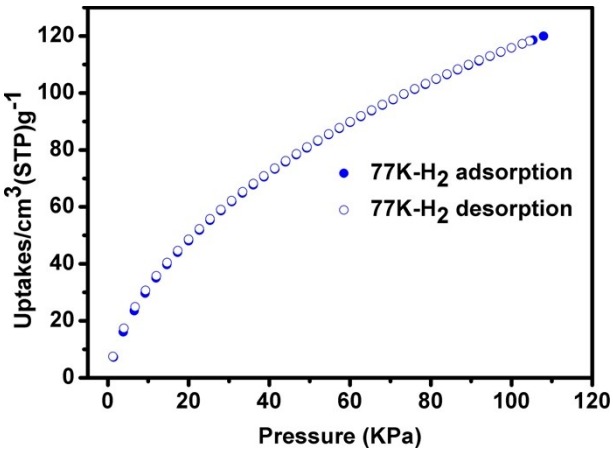

Figure S5 H_2 sorption isotherms for **FJI-H26** at 77K.

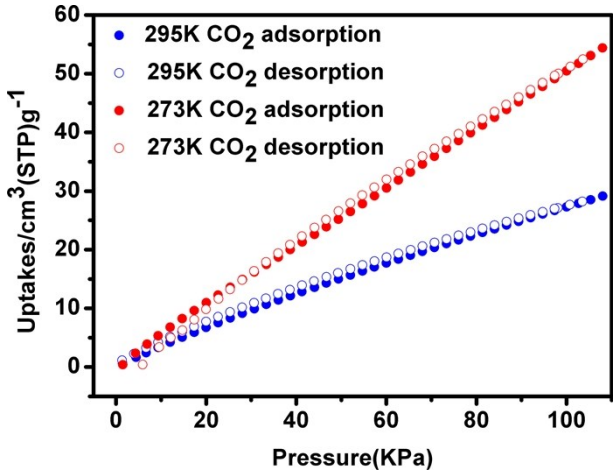

Figure S6. CO_2 sorption isotherms for **FJI-H26** at 273K and 295K.

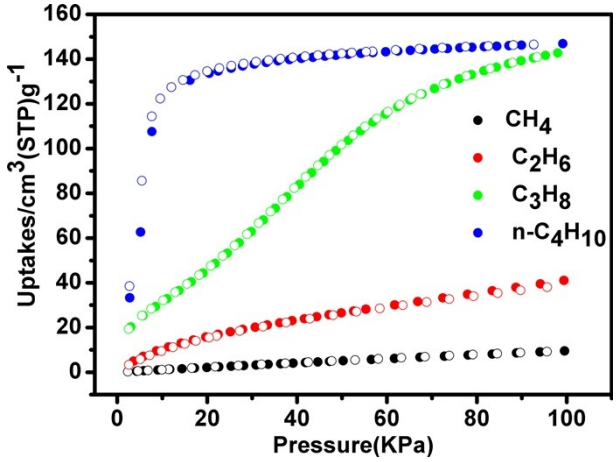

Figure S7. Light hydrocarbons sorption isotherms for **FJI-H26** at 295K.

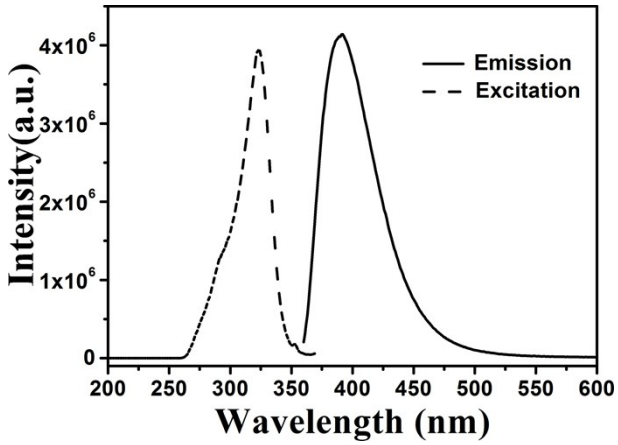

Figure S8. Excitation and emission spectrum of **FJI-H26**.

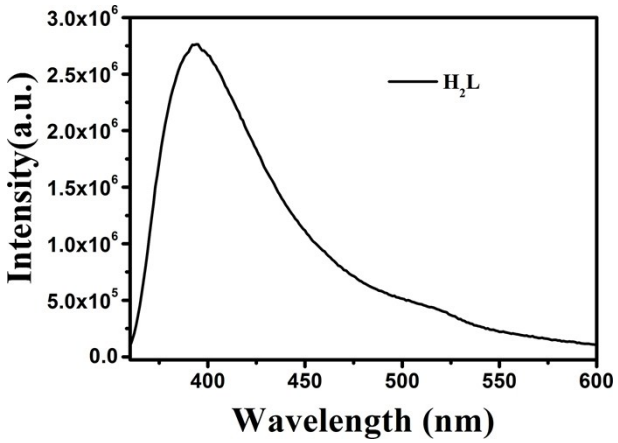

Figure S9. Emission spectrum of ligand under λ_{ex}=329 nm.

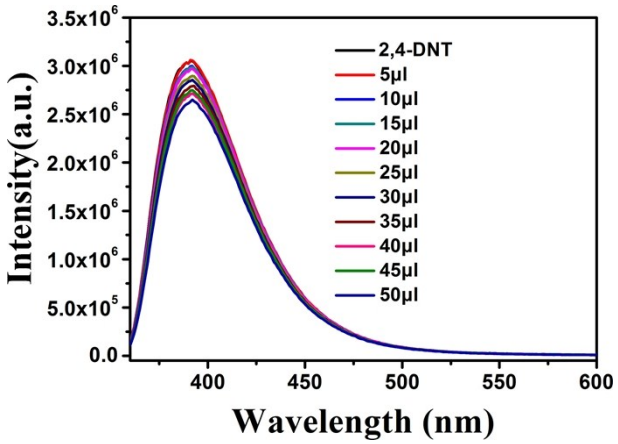

Figure S10. Fluorescence quenching of **FJI-H26** when gradually adding 2,4-DNT.

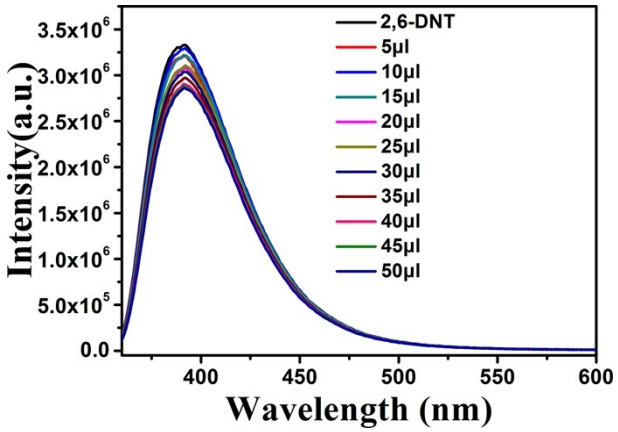

Figure S11. Fluorescence quenching of **FJI-H26** when gradually adding 2,6-DNT.

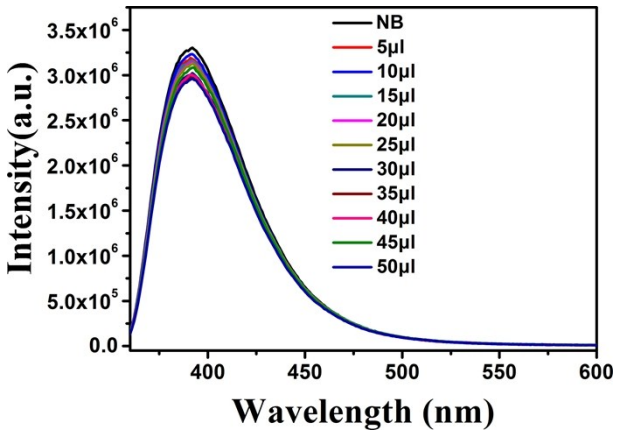

Figure S12. Fluorescence quenching of **FJI-H26** when gradually adding NB.

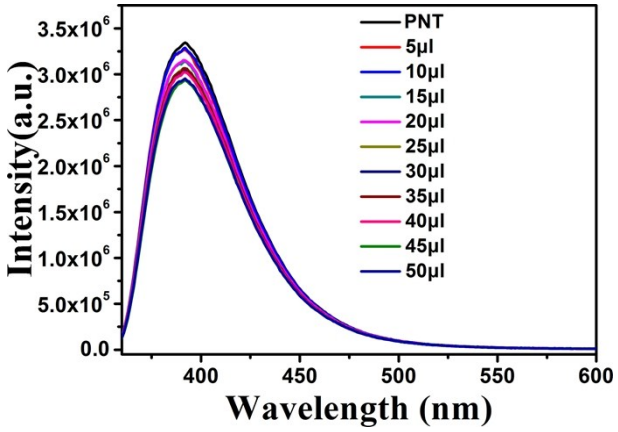

Figure S13. Fluorescence quenching of **FJI-H26** when gradually adding PNT.

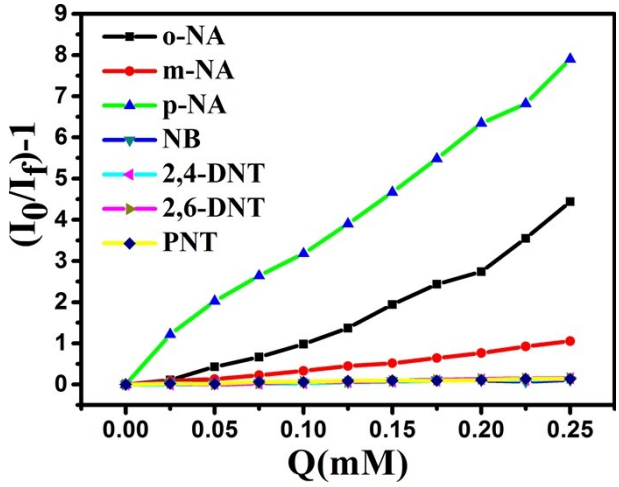

Figure S14. Stern-Volmer (SV) plots for various nitroaromatics dispersed in DMF.

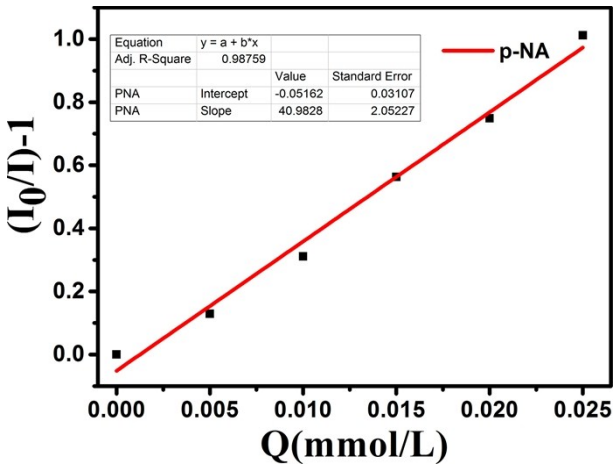

Figure S15. Ksv of p-NA.

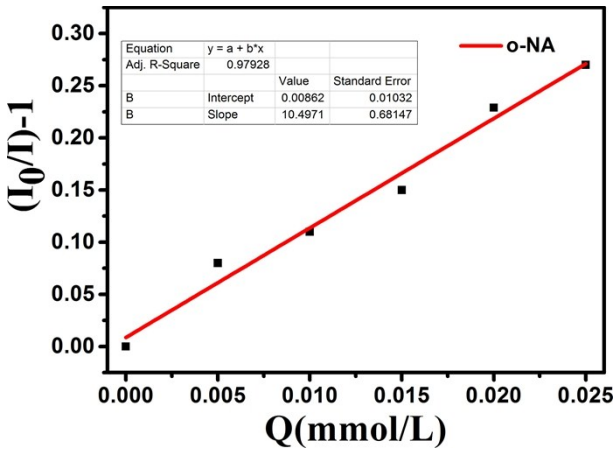

Figure S16. Ksv of o-NA.

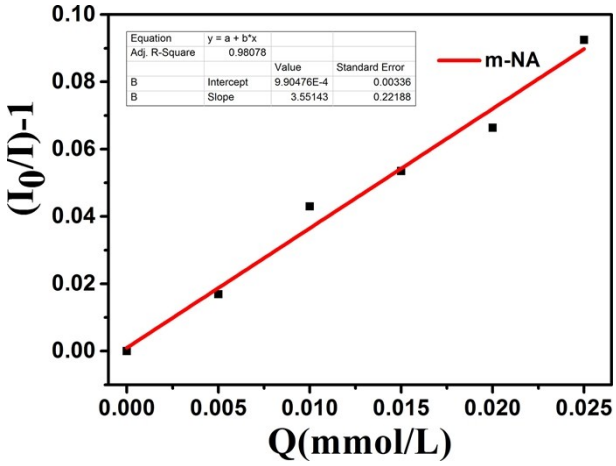

Figure S17. Ksv of m-NA.

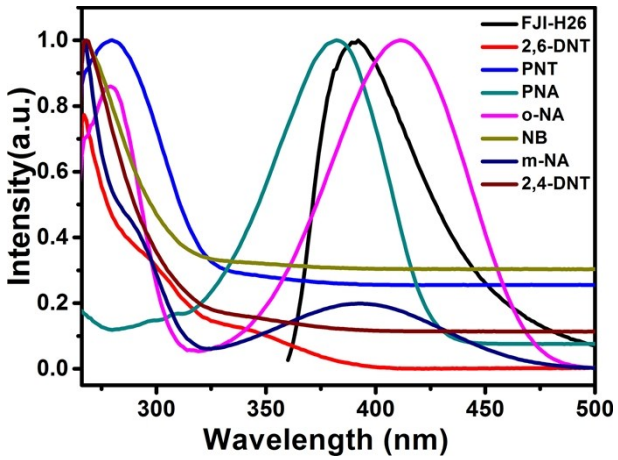

Figure S18. Emission spectrum of **FJI-H26** and UV absorption spectra of different analytes.

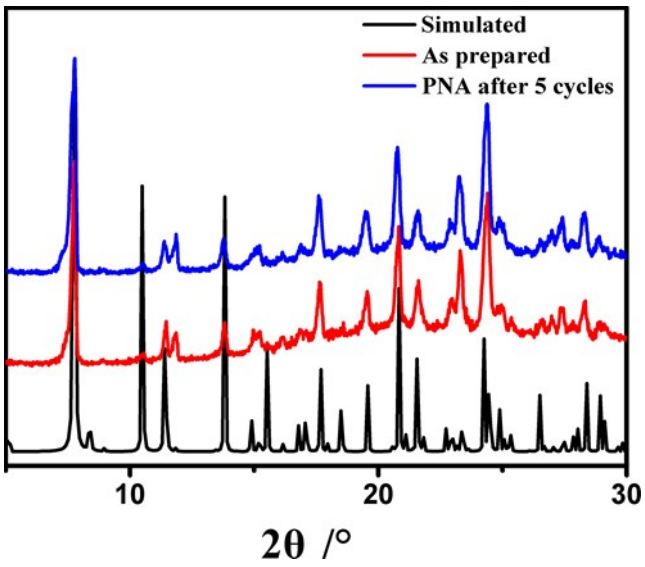

Figure S19. PXRD patterns of **FJI-H26** after 5 cycles fluorescence sensing of *p*-NA.

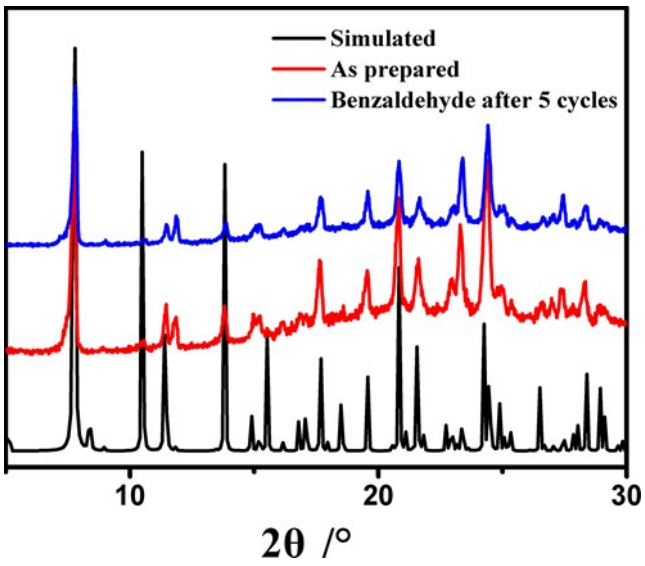

Figure S20. PXRD patterns of **FJI-H26** after 5 cycles fluorescence sensing of benzaldehyde.

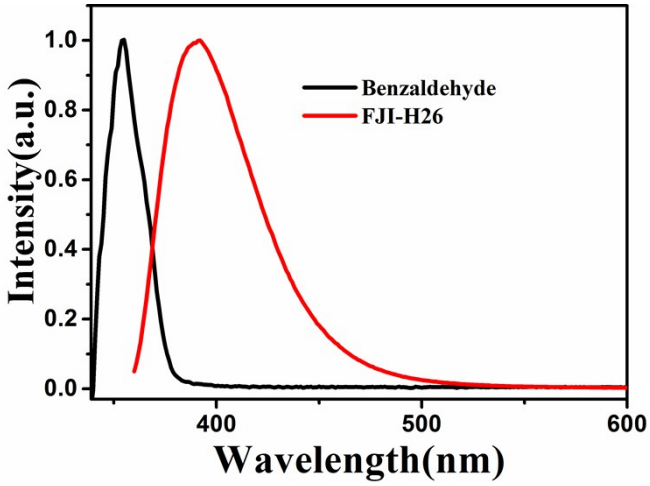

Figure S21. Spectral overlap between normalized absorbance spectra of benzaldehyde and the normalized emission spectra of **FJI-H26**.

Table S1 Crystal data and refinement results for compound **FJI-H26**.

Formula	$C_{18}H_{10}N_6O_4Zn$
Formula weight	439.69
Crystal system	Hexagonal
space group	$P6_222$
a (Å)	22.795 (5)
b (Å)	22.795 (5)
c (Å)	12.477 (4)
α (°)	90
β (°)	90
γ (°)	120
Volume (Å^3)	5615

T (K)	293
Z	6
F (000)	1332
R_1 (I>2σ(I))	0.0497
wR_2 (reflections)	0.1428
Goodness of fit on F_2	1.106

Table S2. The band structure for **FJI-H26** and the frontier molecular orbitals for analytes.

		HOMO(eV)	**LUMO (eV)**	**Band Gap (eV)**
MOF	FJI-H26	+0.76	-0.779	1.539
Analytes	o-NA	-6.4117	-2.8372	3.5745
	m-NA	-6.2374	-2.9002	3.3372
	p-NA	-6.4644	-2.5719	3.8925
	NB	-7.5912	-2.4283	5.1629
	2,4-DNT	-7.156	-2.212	4.944
	2,6-DNT	-7.011	-2.125	4.886
	PNT	-7.364	-2.320	5.044
	Benzyl Alcohol	-6.6446	-0.1644	6.4801
	Benzaldehyde	-7.2196	-2.1301	5.0895

Table S3. Approximate sizes for analytes[a].

Analytes	**Molecular size / Å**
o-NA	8.711 × 7.882 × 2.720
m-NA	9.322 × 7.721 × 2.901
p-NA	9.464 × 6.714 × 3.041
NB	3.000 × 7.306 × 8.892
2,4-DNT	3.000 × 8.535 × 9.898

2,6-DNT	8.177 × 8.345× 8.892
PNT	4.527 × 7.299 × 9.750
Benzyl Alcohol	9.394 × 7.156 × 4.126
Benzaldehyde	8.863 × 7.079 × 3.400

[a]All molecular sizes were performed by using multiwfn software.

Refs:

1. Tian Lu, Feiwu Chen, Multiwfn: A Multifunctional Wavefunction Analyzer, *J. Comput. Chem.* **2012**, 33, 580-592.
2. Humphrey, W., Dalke, A. and Schulten, K., VMD - Visual Molecular Dynamics, *J. Molec. Graphics* **1996**, 14.1, 33-38.