Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Metal-organic frameworks assembled from flexible alicyclic carboxylate and bipyridyl ligands for sensing of nitroaromatic explosives

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Table S1. Crystallographic Data for Compounds **1-3**.

Compounds	1	2	3
Empirical formula	$C_{20}H_{24}O_5N_2Cd$	$C_{20}H_{22}O_4N_2Ni$	$C_{42}H_{48}O_8N_4Cd_2$
Formula mass	484.81	413.11	961.64
Crystal system	Orthorhombic	Orthorhombic	Triclinic
Space group	$Pna2_1$	$Pna2_1$	P-1
a (Å)	8.7092(7)	15.997(6)	10.0056(5)
b (Å)	17.5095(15)	10.429(4)	10.2640(5)
c (Å)	12.4774(10)	11.462(4)	22.7508(10)
α (°)	90	90	84.883(4)
β (°)	90	90	81.606(4)
γ (°)	90	90	63.403(5)
***V* (Å^3)**	1902.7(3)	1912.2(13)	2066.07(17)
Z	4	4	2
***D*$_{calc}$ (g·cm^{-3})**	1.692	1.435	1.546
Reflections collected	15651	15426	14665
Data [I>2σ(I)]/parameters	4214/253	4132/244	8095/568
Goodness-of-fit on F^2	1.198	1.009	1.014
Flack parameter	0.56(3)	0.02(2)	
R$_1$ indices (I > 2σ(I))	0.0237	0.0557	0.0450
wR$_2$ indices (all data)	0.0834	0.1101	0.1179
Residual electron density	0.520	0.774	0.970

[a] $R = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. [b] $wR(F^2) = [\Sigma w(Fo^2 - Fc^2)^2/\Sigma w(Fo^2)^2]^{1/2}$.

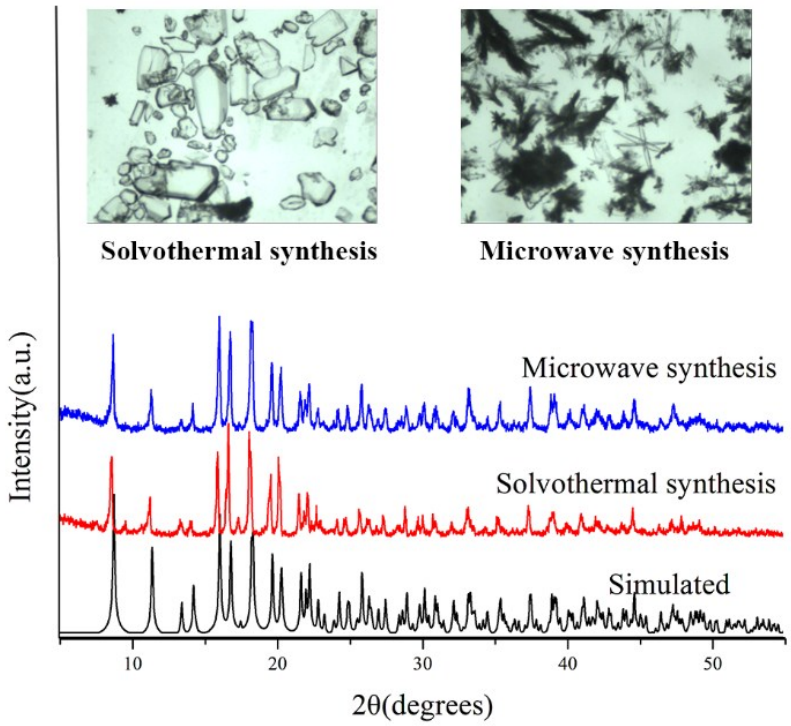

Fig. S1 Comparison PXRD of compound **1** prepared from microwave-assisted heating (blue) and solvothermal synthesis (red) (inserted: optical microscope images of **1**).

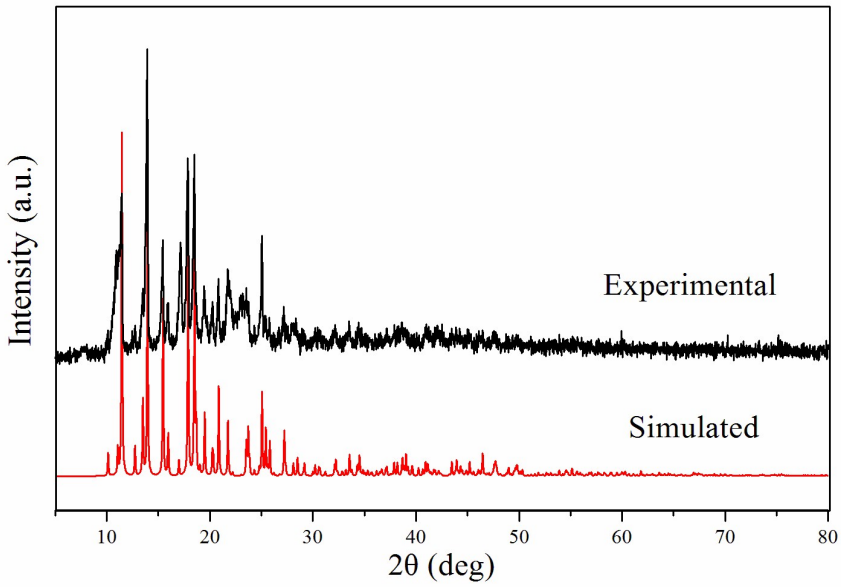

Fig. S2 PXRD of as-synthesized sample of compound **2**.

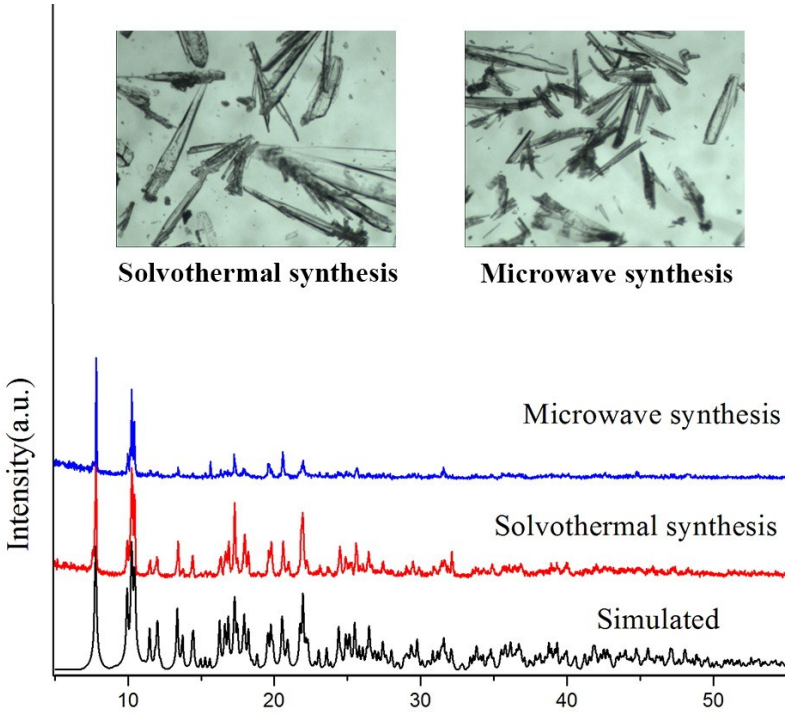

Fig. S3 Comparison PXRD of compound **3** prepared from microwave-assisted heating (blue) and solvothermal synthesis (red) (inserted: optical microscope images of **3**).

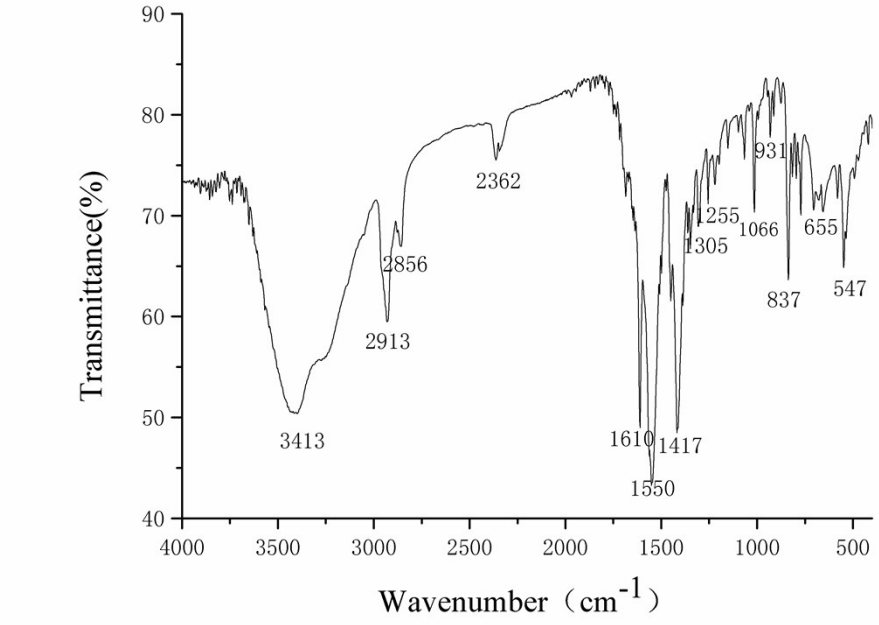

Fig. S4 FT-IR spectrum for compound **1**.

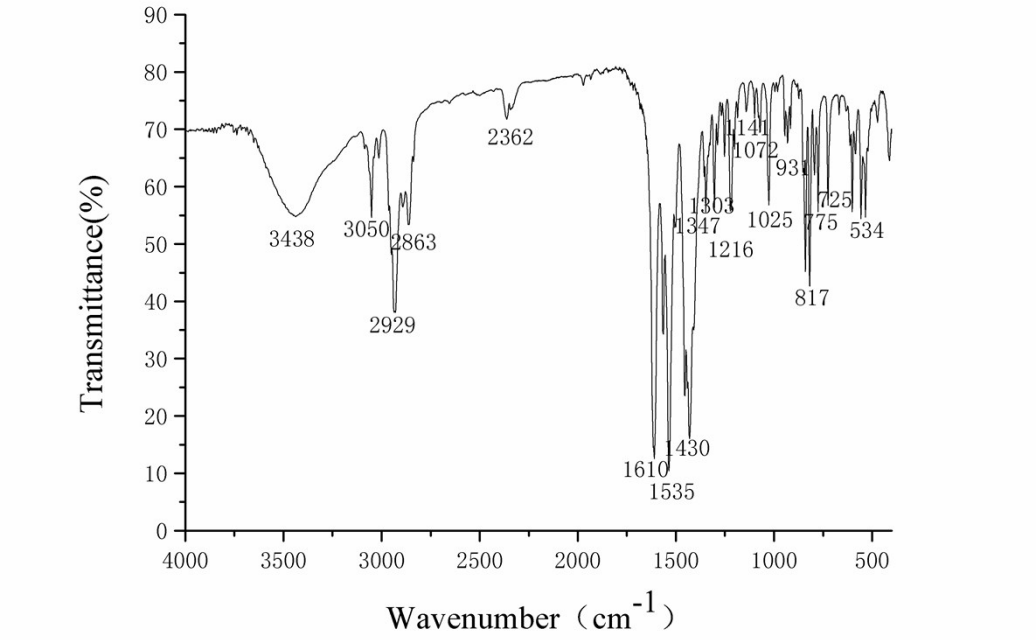

Fig. S5 FT-IR spectrum for compound **2**.

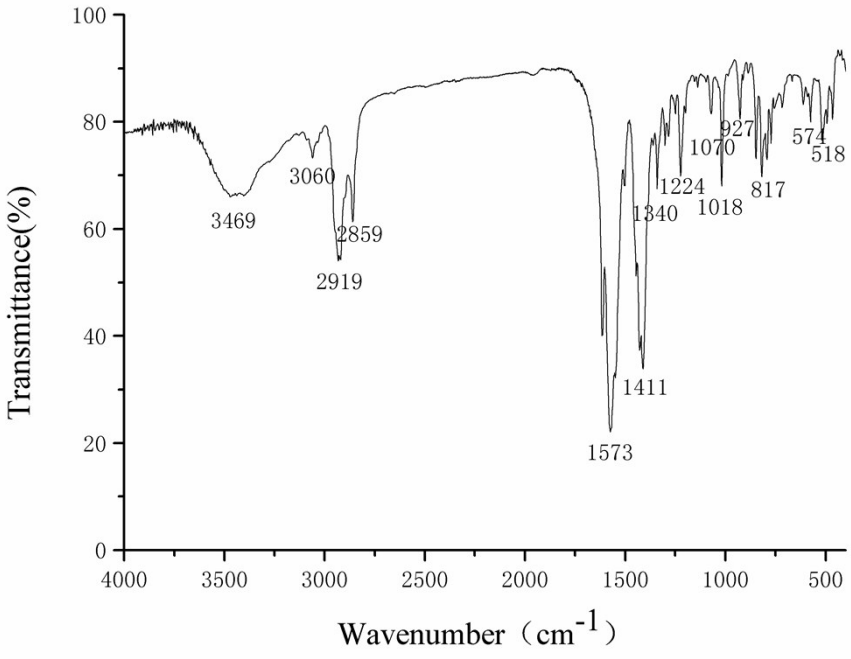

Fig. S6 FT-IR spectrum for compound **3**.

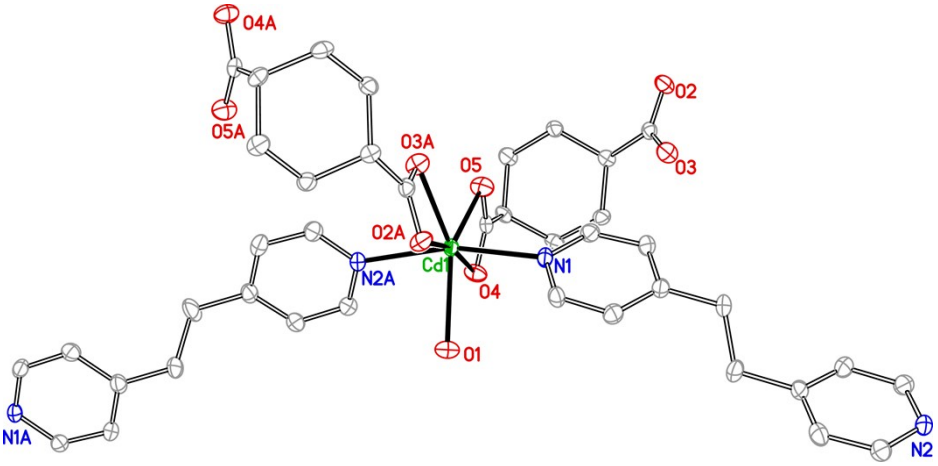

Fig. S7 ORTEP representation of the coordination environment of metal ion in compound **1** with thermal ellipsoids at 30% probability level.

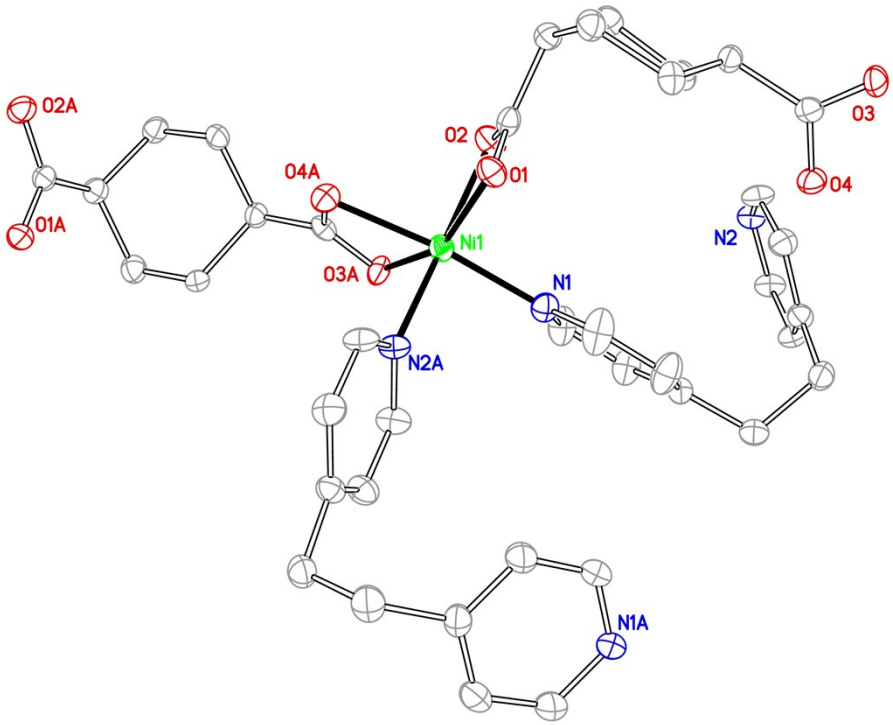

Fig. S8 ORTEP representation of the coordination environment of metal ion in compound **2** with thermal ellipsoids at 30% probability level.

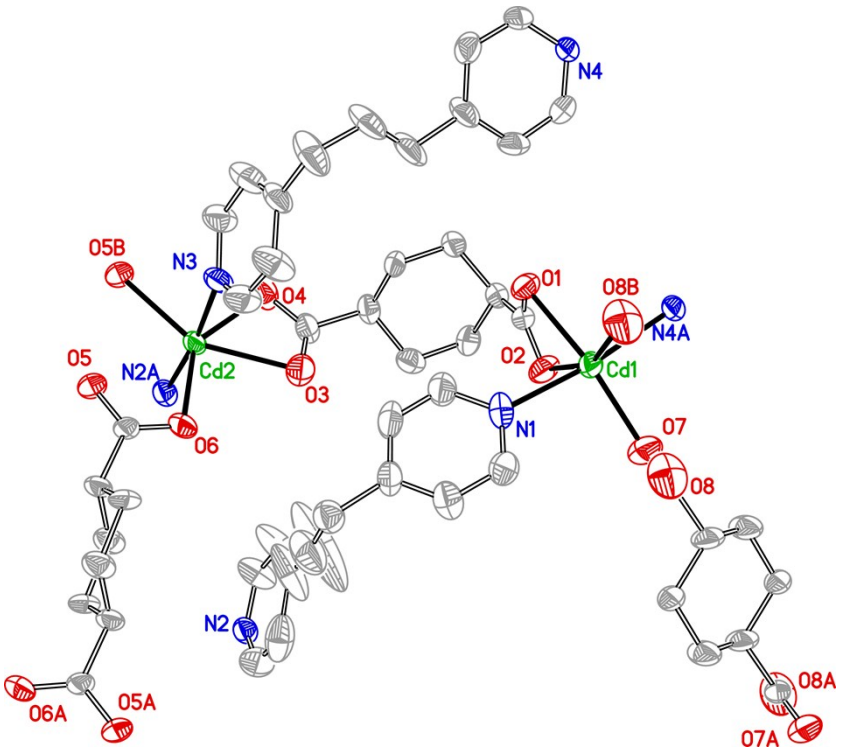

Fig. S9 ORTEP representation of the coordination environment of metal ion in compound **3** with thermal ellipsoids at 30% probability level.

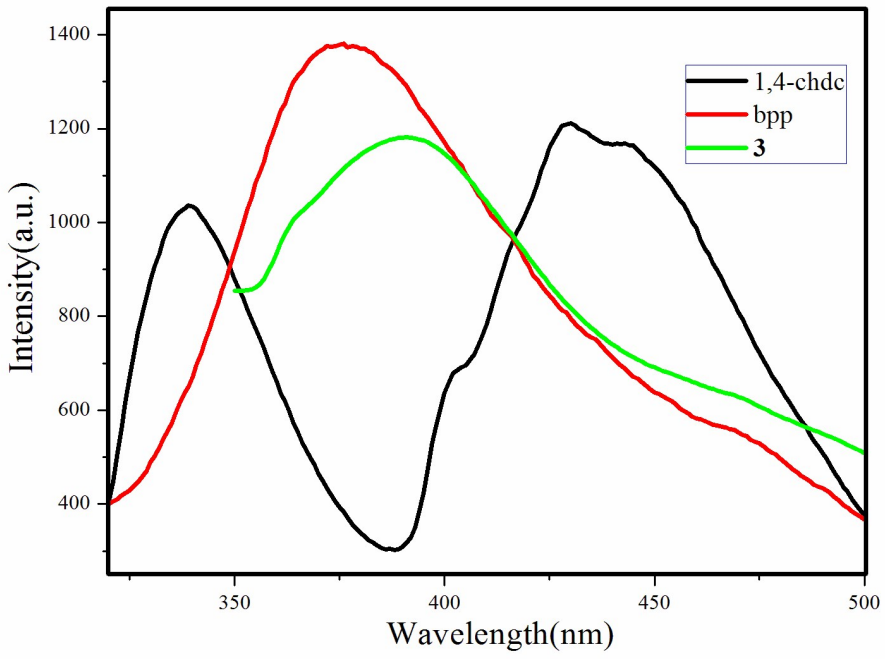

Fig. S10 Solid-state emission spectrum for free ligands and compound **3**.

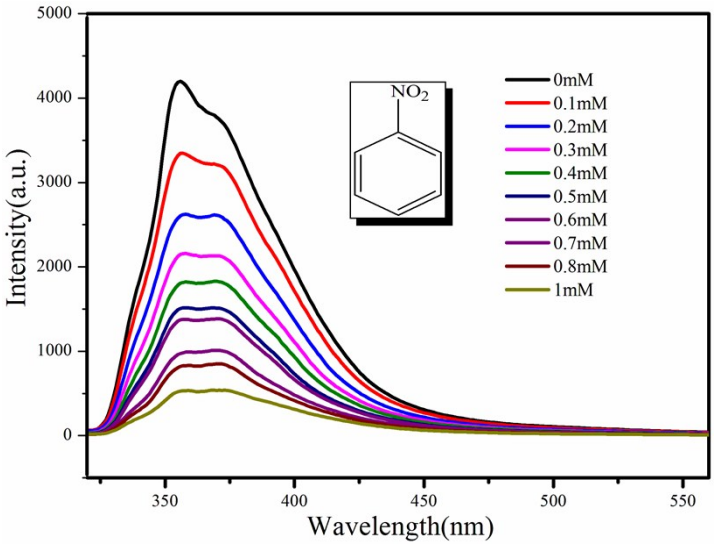

Fig.S11 The fluorescence titration of compound **1** upon incremental addition of NB solution in DMF.

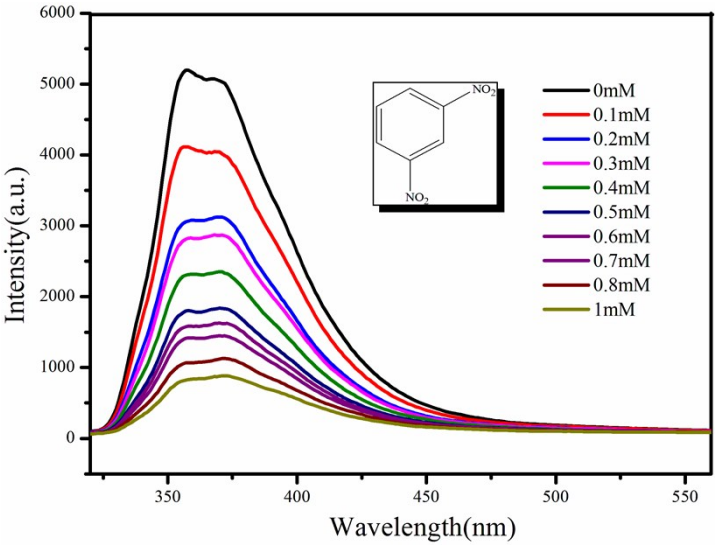

Fig.S12 The fluorescence titration of compound **1** upon incremental addition of 1,3-DNB solution in DMF.

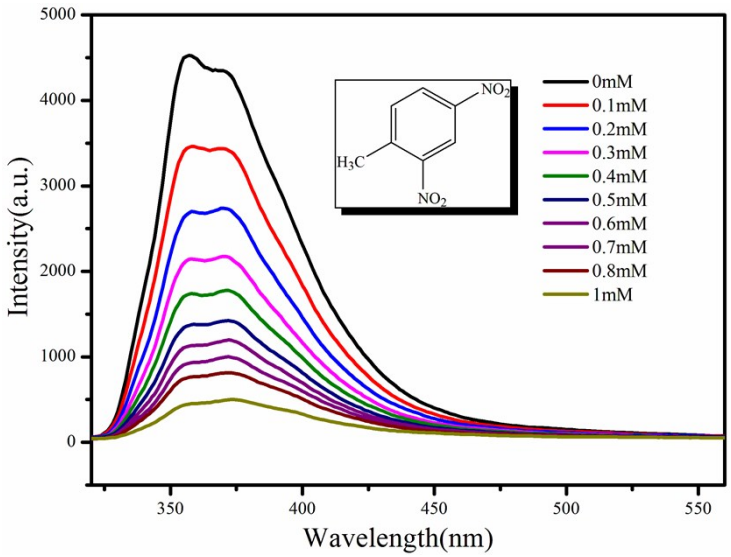

Fig.S13 The fluorescence titration of compound **1** upon incremental addition of 2,4-DNT solution in DMF.

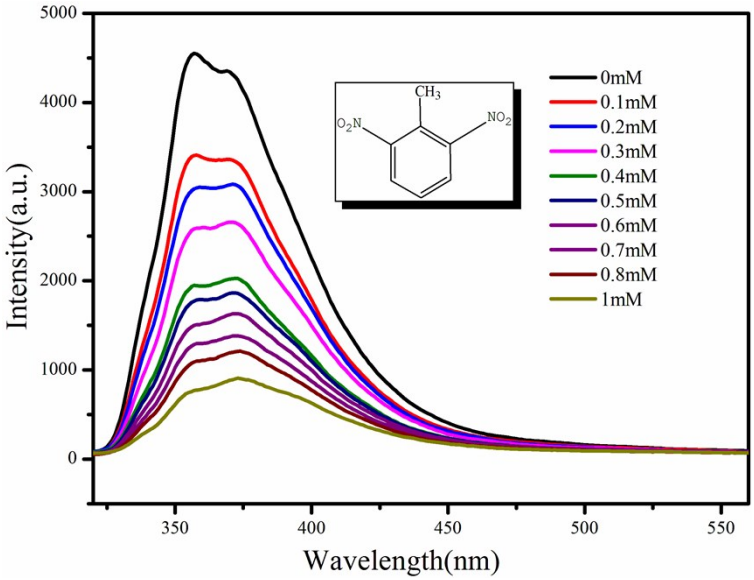

Fig.S14 The fluorescence titration of compound **1** upon incremental addition of 2,6-DNT solution in DMF.

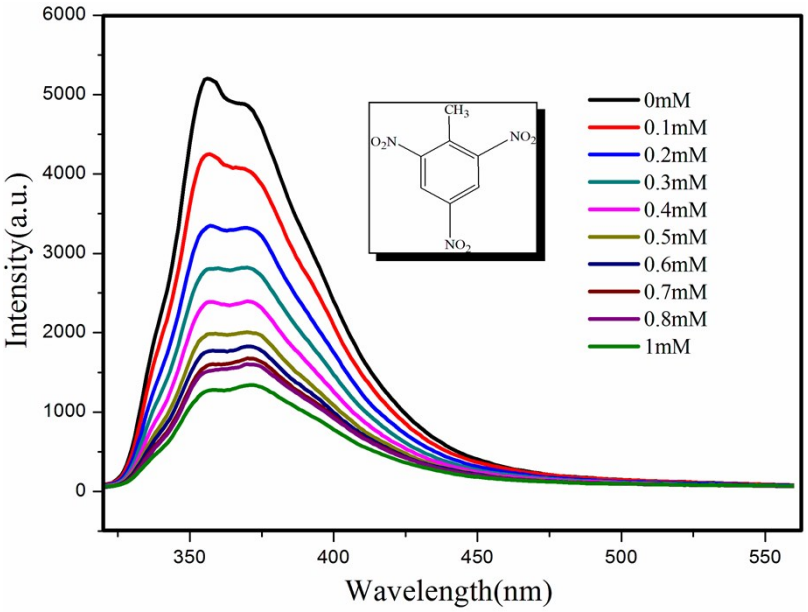

Fig.S15 The fluorescence titration of compound **1** upon incremental addition of TNT solution in DMF.

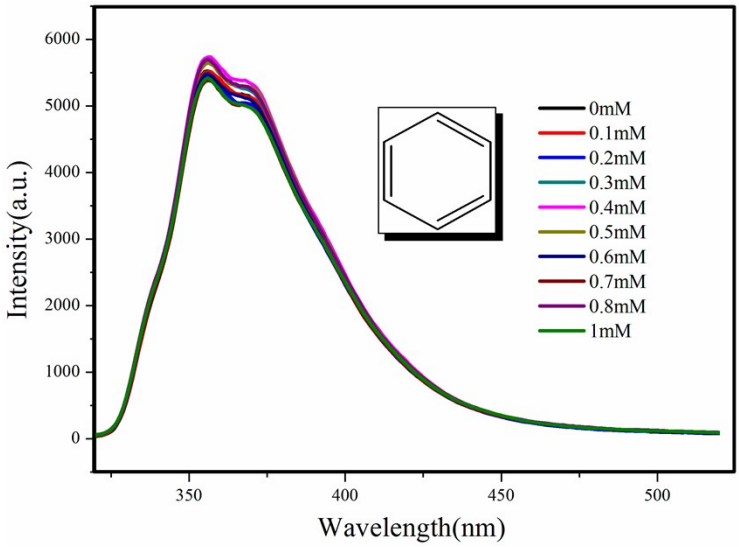

Fig.S16 The fluorescence titration of compound **1** upon incremental addition of benzene solution in DMF.

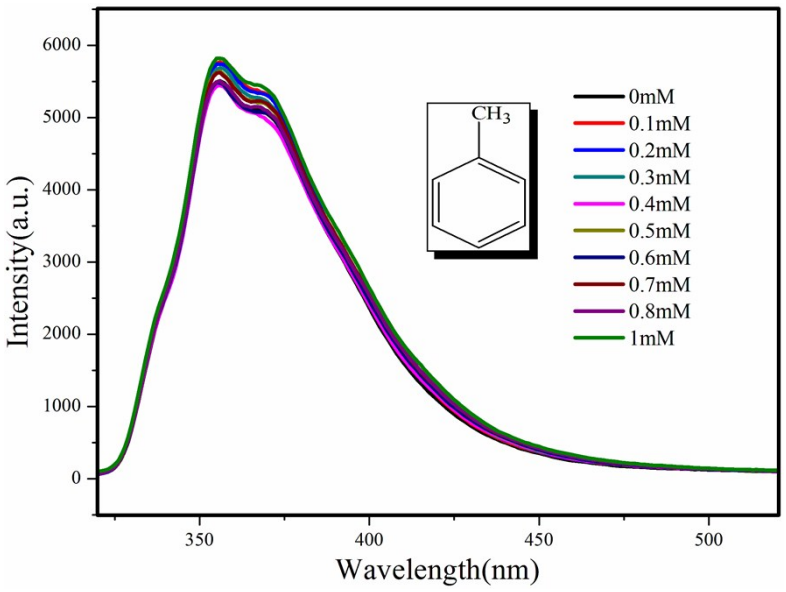

Fig.S17 The fluorescence titration of compound **1** upon incremental addition of toluene solution in DMF.

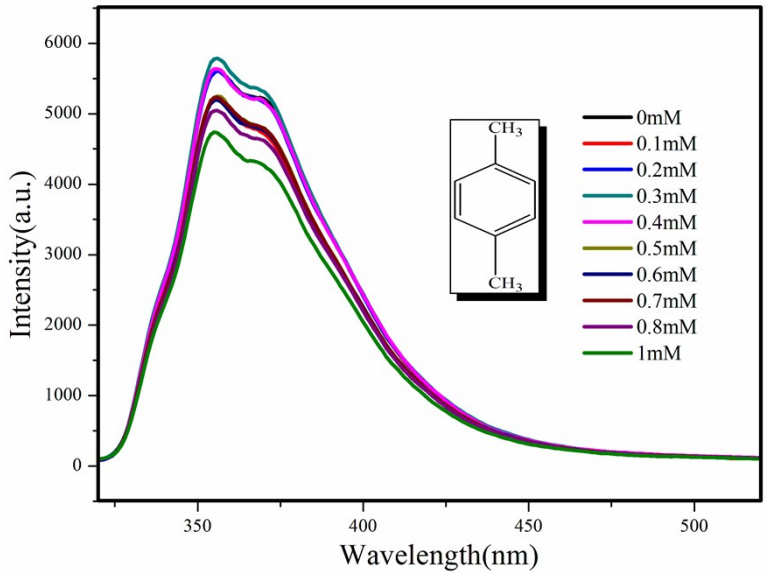

Fig.S18 The fluorescence titration of compound **1** upon incremental addition of p-xylene solution in DMF.

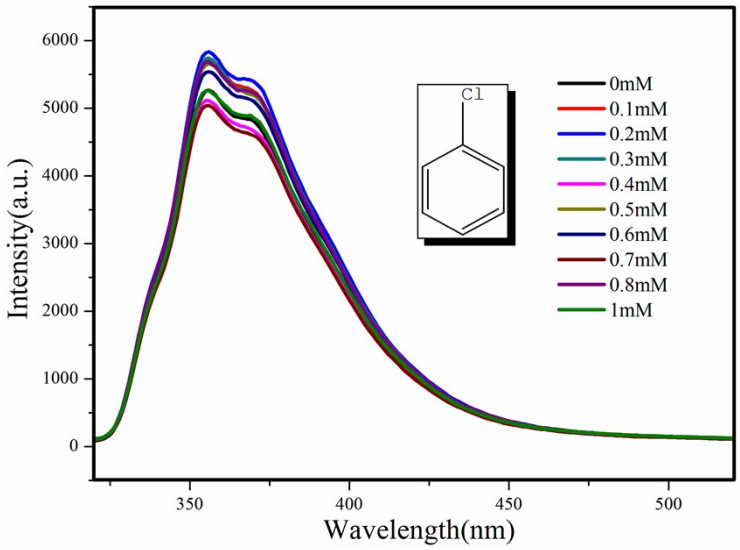

Fig.S19 The fluorescence titration of compound **1** upon incremental addition of chlorobenzene solution in DMF.

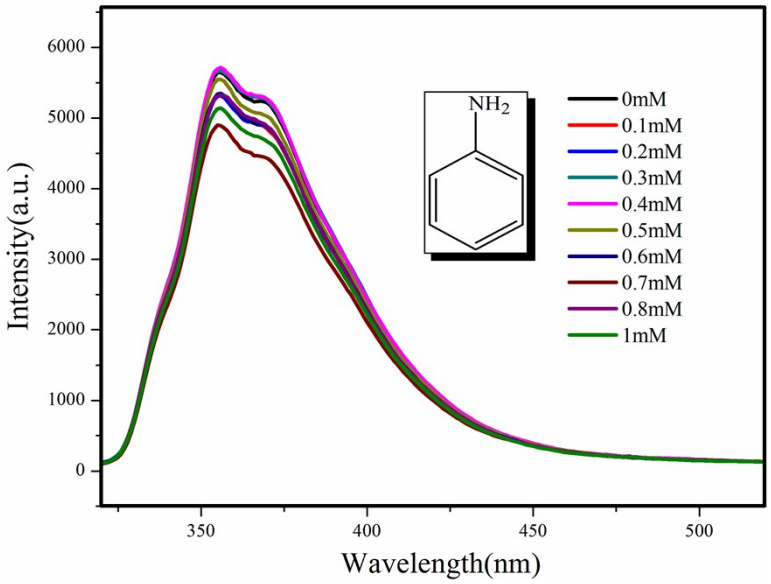

Fig.S20 The fluorescence titration of compound **1** upon incremental addition of phenol solution in DMF.

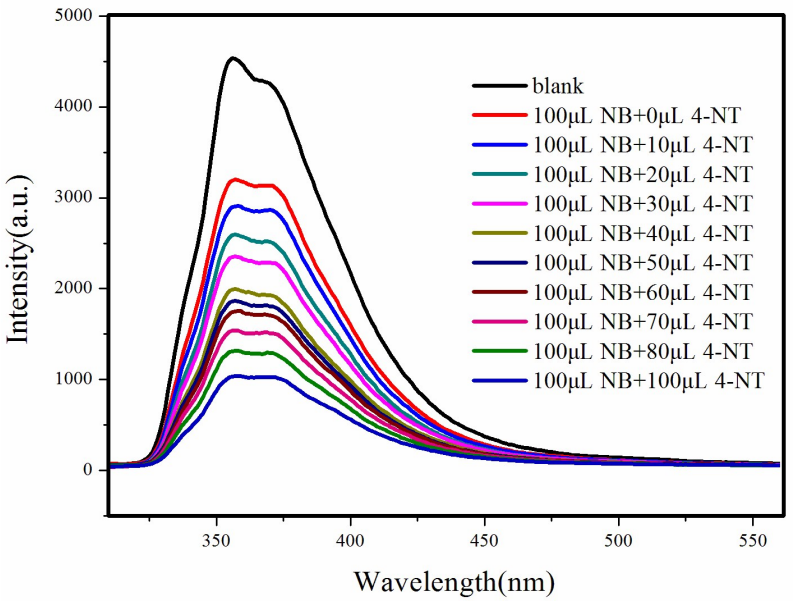

Fig.S21 The fluorescence emission spectra of compound **1** upon firstly added 100 μL 2 mM NB followed by incremental 2 mM 4-NT solution.

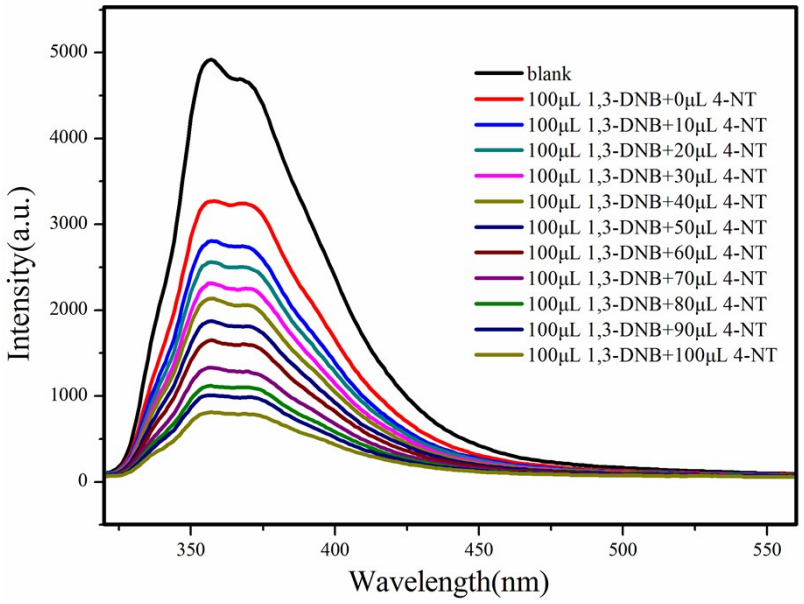

Fig.S22 The fluorescence emission spectra of compound **1** upon firstly added 100 μL 2 mM 1,3-DNB followed by incremental 2 mM 4-NT solution.

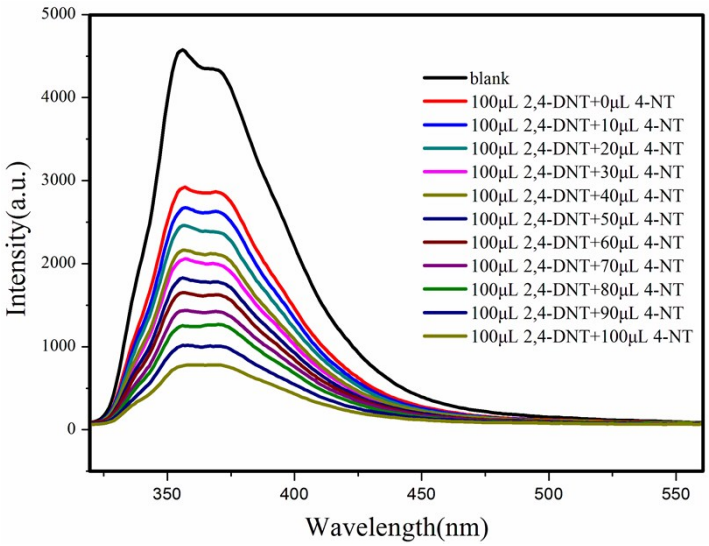

Fig.S23 The fluorescence emission spectra of compound **1** upon firstly added 100 μL 2 mM 2,4-DNT followed by incremental 2 mM 4-NT solution.

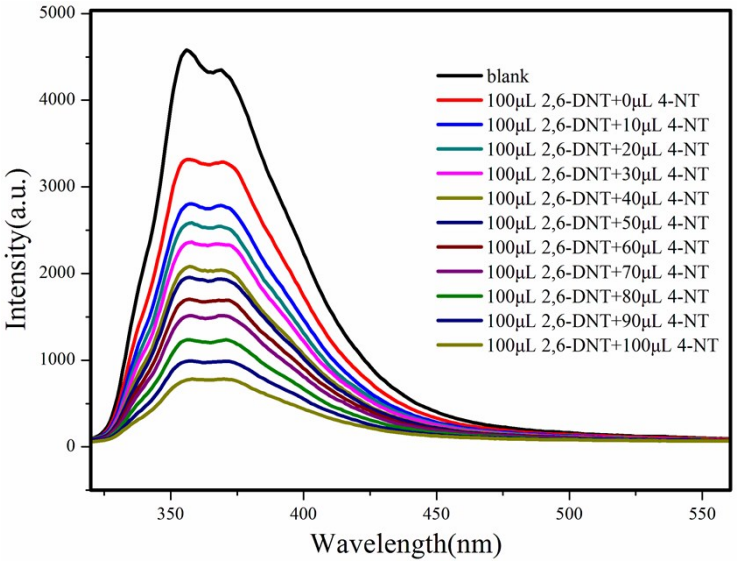

Fig.S24 The fluorescence emission spectra of compound **1** upon firstly added 100 μL 2 mM 2,6-DNT solution followed by incremental 2 mM 4-NT solution.

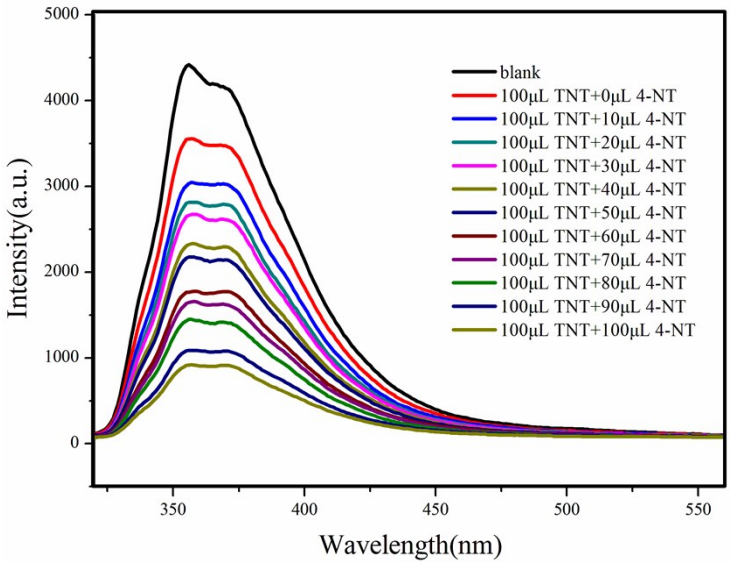

Fig.S25 The fluorescence emission spectra of compound **1** upon firstly added 100 μL 2 mM TNT followed by incremental 2 mM 4-NT solution.

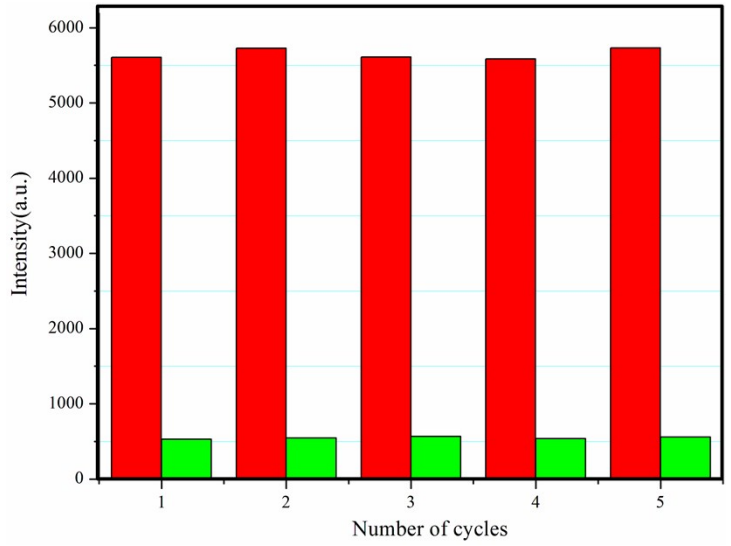

Fig.S26 Reproducibility of compound **1** dispersed in DMF in the presence of 4-NT. The red bars represent the original fluorescence intensity and green bars represent the intensity upon addition of 0.5 mM 4-NT.

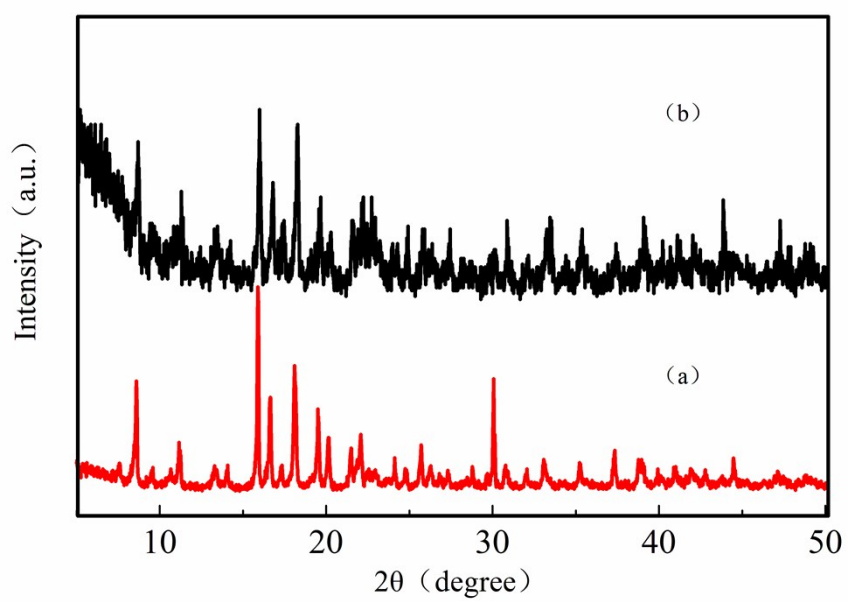

Fig.S27 Comparison of PXRD of the as-made sample of **1** (red) and **1'** which is quenched by 4-NT and then washed with DMF (black).