Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Solvent-induced construction of two zinc metal-organic frameworks with high selective detection for nitroaromatic explosives

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Table S1 Crystal Data and Structure Refinement for **1** and **2.**

Compound	**1**	**2**
Formula	C_{98} $H_{79}N_5O_{28}$ Zn_6	$C_{26}H_{26}N_2O_7Zn$
Fw	2167.14	543.90
Temp (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Cryst syst	Monoclinic, *C2/c*	Orthorhombic, *Pbcn*
a (Å)	a = 19.953(7)	a = 16.7153(8)
b (Å)	b = 9.495(4)	b = 8.4558(4)
c (Å)	c = 25.805(10)	c = 35.4943(17)
*V (*Å^3*)*	4886(3)	5016.8(4)
Z	2	8
F(000)	2054	2048
θ range (deg)	1.58 -26.44	1.67 -28.30
reflns collected / unique	8006 / 4843	34683 / 6234
R_{int}	0.0621	0.0557
data / restraints /params	4843 / 0 / 318	6234 / 0 / 325
GOF on F^2	1.076	1.044
R_1, wR_2 [$I>2\sigma(I)$]	0.0943, 0.2531	0.0576, 0.1656
R_1, wR_2 (all data)	0.1522, 0.2925	0.0822, 0.1809

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$.

Table S2 Selected bond lengths [Å] and angles [°] for **1**.

Zn(1)-O(3)#1	1.951(3)	Zn(2)-O(6)#4	2.112(4)
Zn(1)-O(2)#2	1.979(4)	Zn(2)-O(7)#5	2.157(4)
Zn(1)-O(4)#3	1.981(4)	Zn(2)-O(7)#6	2.157(4)
Zn(1)-O(1)	2.030(4)	O(2)-Zn(1)#7	1.979(4)
Zn(2)-O(5)	2.109(4)	O(3)-Zn(1)#1	1.951(3)
Zn(2)-O(5)#4	2.109(4)	O(4)-Zn(1)#3	1.981(4)
Zn(2)-O(6)	2.112(4)	O(7)-Zn(2)#6	2.157(4)
O(3)#1-Zn(1)-O(2)#2	130.78(17)	O(6)-Zn(2)-O(6)#4	179.998(1)
O(3)#1-Zn(1)-O(4)#3	115.76(15)	O(5)-Zn(2)-O(7)#5	90.00(17)
O(2)#2-Zn(1)-O(4)#3	108.41(17)	O(5)#4-Zn(2)-O(7)#5	90.00(17)
O(3)#1-Zn(1)-O(1)	92.17(14)	O(6)-Zn(2)-O(7)#5	94.68(16)
O(2)#2-Zn(1)-O(1)	93.79(16)	O(6)#4-Zn(2)-O(7)#5	85.32(16)
O(4)#3-Zn(1)-O(1)	108.31(14)	O(5)-Zn(2)-O(7)#6	90.00(17)
O(5)-Zn(2)-O(5)#4	180	O(5)#4-Zn(2)-O(7)#6	90.00(17)
O(5)-Zn(2)-O(6)	88.06(16)	O(6)-Zn(2)-O(7)#6	85.32(16)
O(5)#4-Zn(2)-O(6)	91.94(16)	O(6)#4-Zn(2)-O(7)#6	94.68(16)
O(5)-Zn(2)-O(6)#4	91.94(16)	O(7)#5-Zn(2)-O(7)#6	180.0(2)
O(5)#4-Zn(2)-O(6)#4	88.06(16)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 -x+1/2,y+1/2,-z+1/2

#3 -x,-y+1,-z+1 #4 -x-1/2,-y-1/2,-z+1

#5 x-1/2,-y-1/2,z+1/2 #6 -x,y,-z+1/2

#7 -x+1/2,y-1/2,-z+1/2

Table S3 Selected bond lengths [Å] and angles [°] for **2**.

Zn(1)-O(2)#1	1.9505(18)	O(2)-Zn(1)#1	1.9503(18)
Zn(1)-O(3)#2	1.9514(19)	O(3)-Zn(1)#4	1.9514(19)
Zn(1)-O(4)#3	1.9583(19)	O(4)-Zn(1)#3	1.9583(19)
Zn(1)-O(1)	2.0031(18)		
O(2)#1-Zn(1)-O(3)#2	124.61(9)	O(2)#1-Zn(1)-O(1)	107.85(8)
O(2)#1-Zn(1)-O(4)#3	112.52(9)	O(3)#2-Zn(1)-O(1)	107.47(8)
O(3)#2-Zn(1)-O(4)#3	106.80(9)	O(4)#3-Zn(1)-O(1)	92.84(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2 #2 -x+3/2,y+1/2,z

#3 -x+1,y,-z+3/2 #4 -x+3/2,y-1/2,z

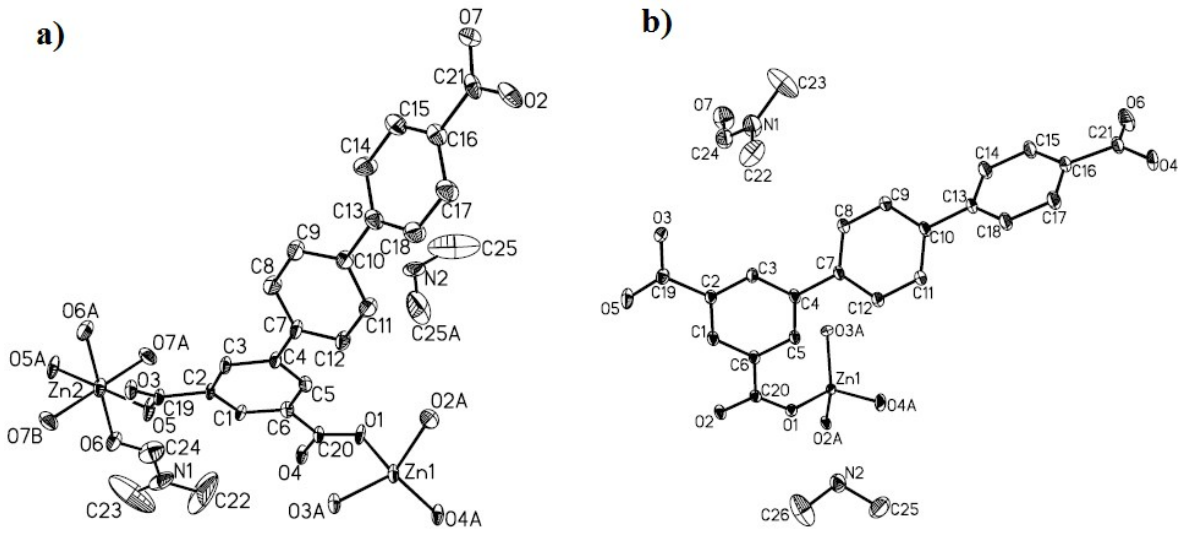

Fig. S1 a), b) The asymmetric unit of **1** and **2** showing ellipsoid at the 30% probability level. The symmetry codes for **1**: O2A: -x+1/2, y+1/2, -z+1/2; O3A: -x, -y, -z+1; O4A: -x, -y+1, -z+1; O5A: -x-1/2, -y-1/2, -z+1; O6A: -x-1/2, -y-1/2, -z+1; O7A: x-1/2, -y-1/2, z+1/2; O7B: -x, y, -z+1/2. The symmetry codes for **2**: O2A: -x+1, -y+1, -z+2; O3A: -x+3/2, y+1/2, z; O4A: -x+1, y, -z+3/2.

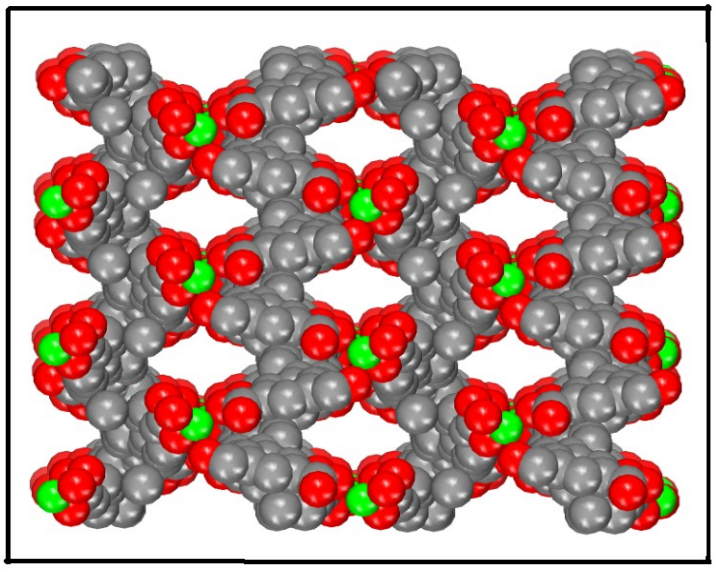

Fig. S2 The space filling structure of **2** showing the channels along [001] direction.

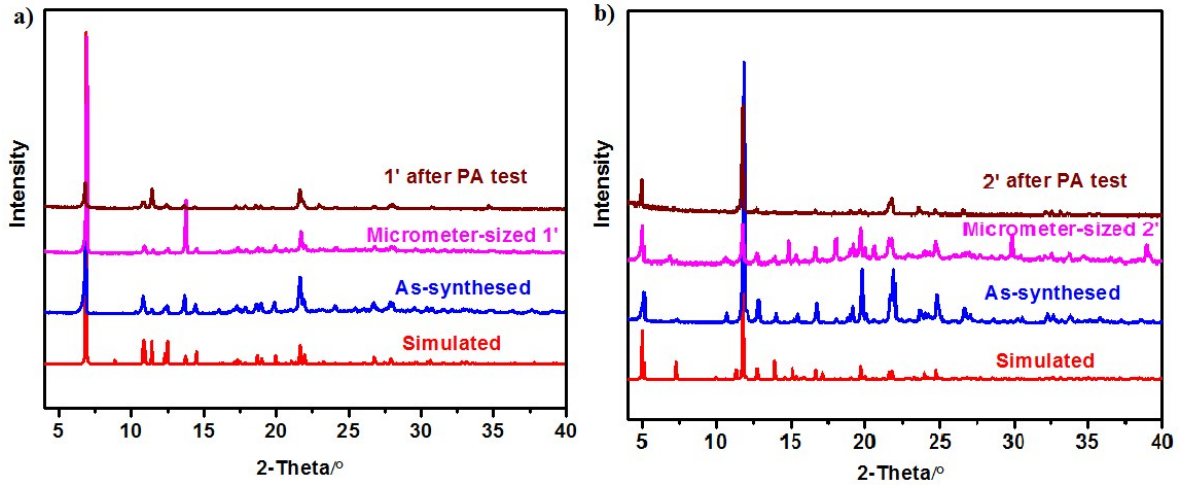

Fig. S3 a), b) XRD patterns of the simulated patterns calculated from the single crystal X-ray data, the as-synthesized, micrometer-sized samples and samples after PA quenching and recovery test for five times of **1'** and **2'**, respectively.

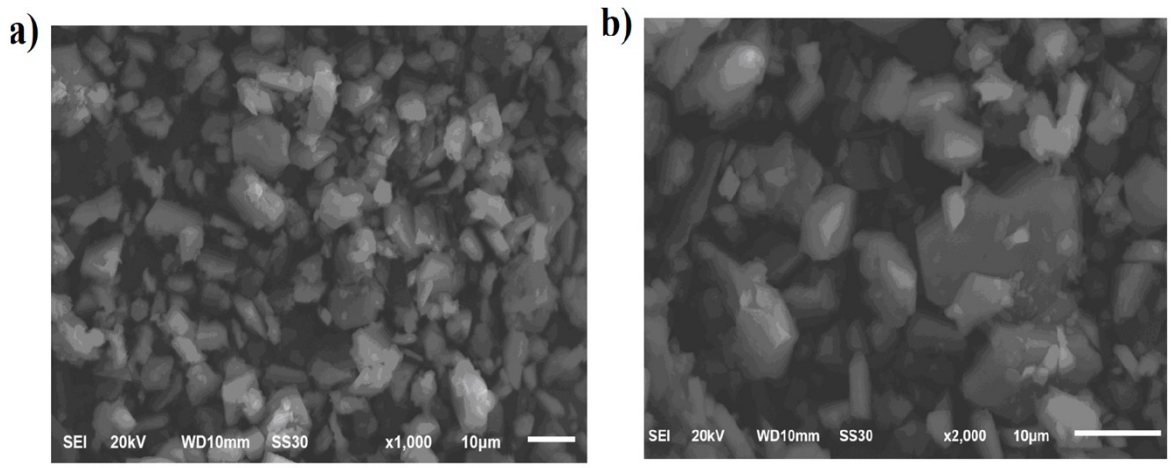

Fig. S4 SEM images of micrometer-sized **1'** and **2'**.

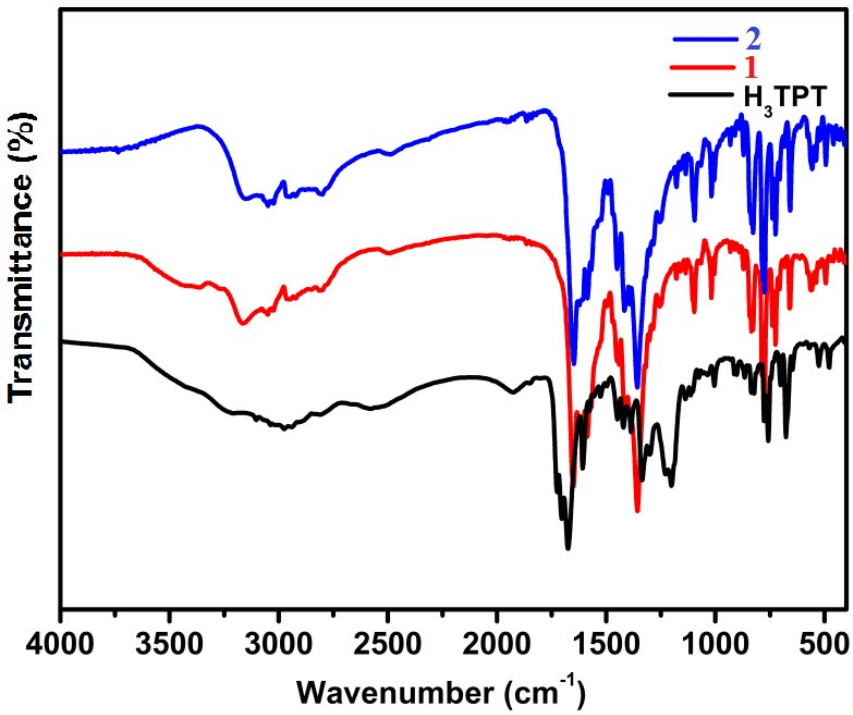

Fig. S5 IR spectra of H_3TPT, **1** and **2**.

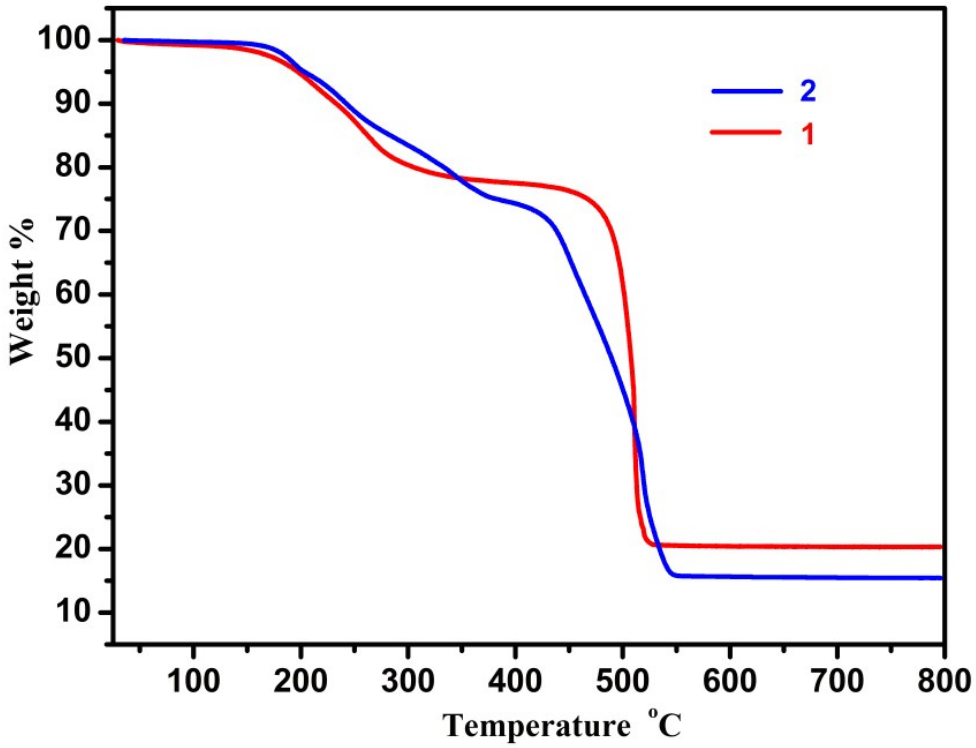

Fig. S6 TG curves of **1** and **2**.

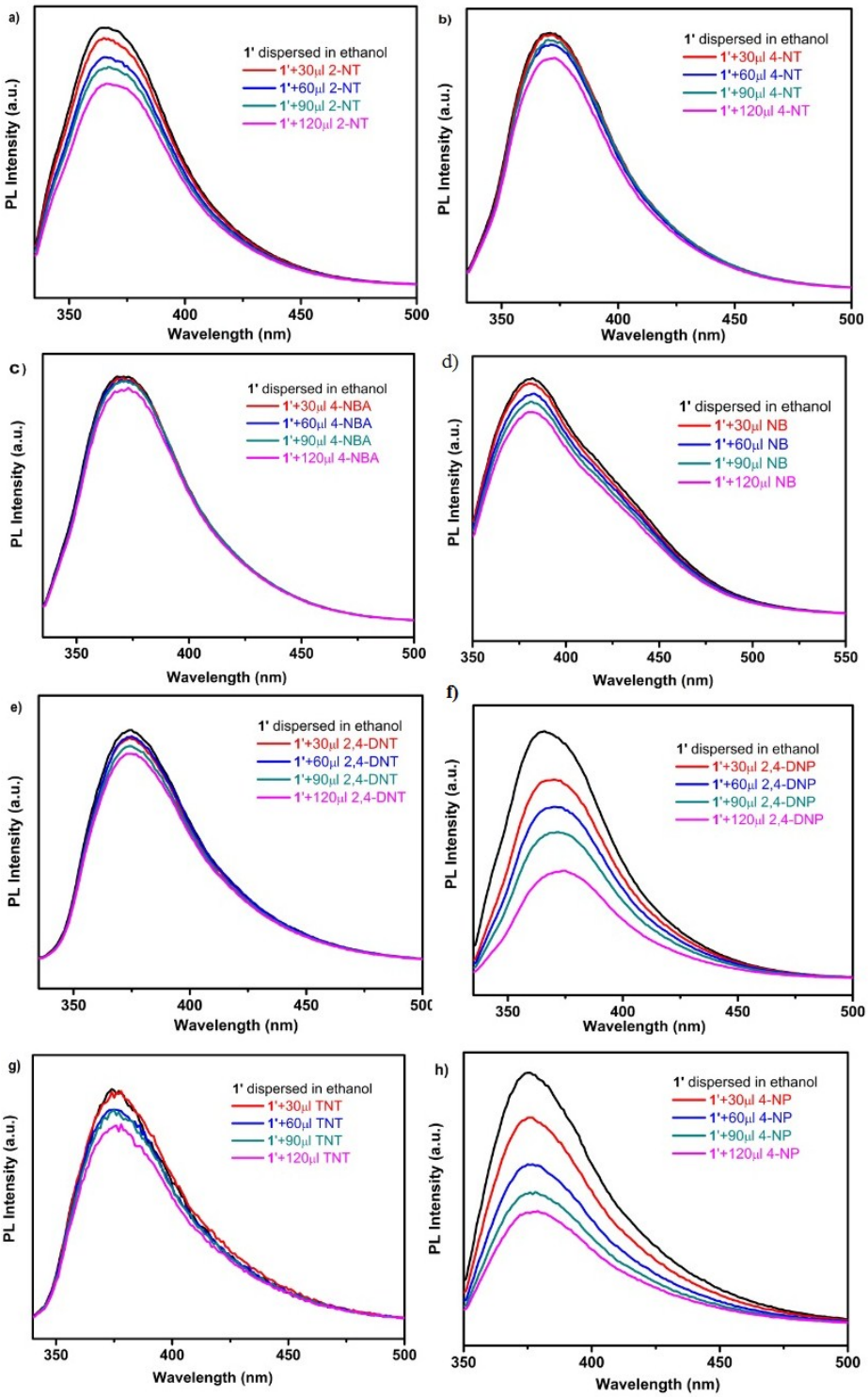

Fig. S7 Fluorescent titrations of 0.5 mg **1'** dispersed in 2 mL ethanol solution with the addition of different volume of 0.001 M solution of a) 2-NT, b) 4-NT, c) 4-NBA, d) NB, e) 2,4-DNT, f) 2,4-DNP, g) TNT, and h) 4-NP in ethanol. The fluorescent emission spectra were recorded from 350 nm to 500 nm upon the excitation at 319 nm.

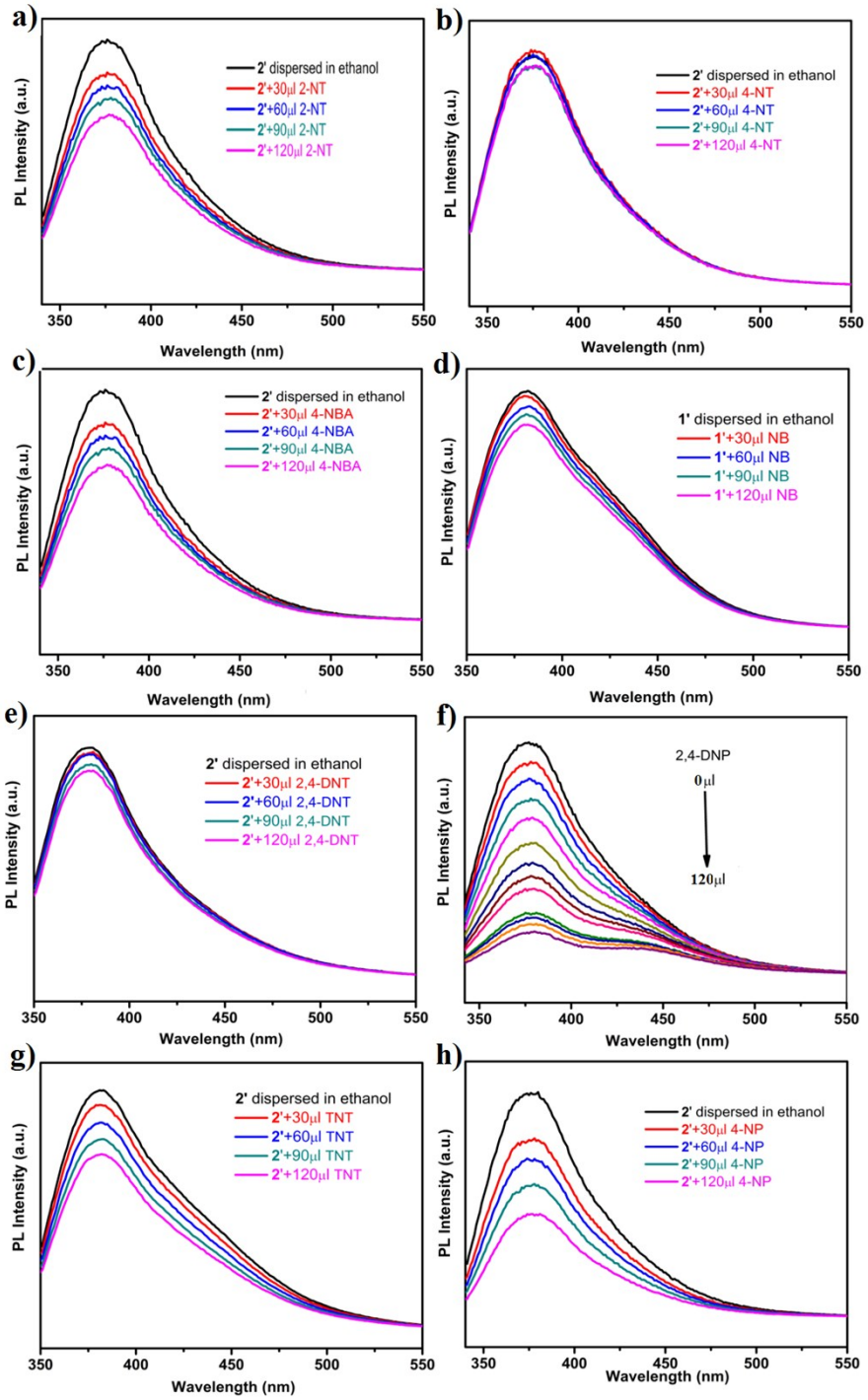

Fig. S8 Fluorescent titrations of 0.5 mg **2'** dispersed in 2 mL ethanol solution with the addition of different volume of 0.001 M solution of a) 2-NT, b) 4-NT, c) 4-NBA, d) NB, e) 2,4-DNT, f) 2,4-DNP, g) TNT, and h) 4-NP in ethanol. The fluorescent emission spectra were recorded from 350 nm to 550 nm upon the excitation at 335 nm.

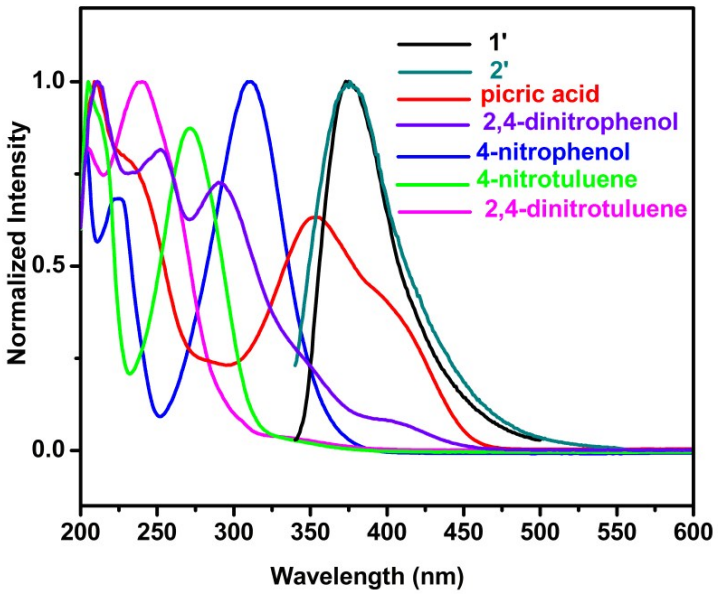

Fig. S9 Spectral overlap between the absorption spectra of NACs and the emission spectra of **1'** and **2'** in ethanol.