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Supporting information for article:

Preparation, characterization and luminescence sensing properties of two Zn^{II} MOFs with mixed 5-amino-2,4,6-tribromo-isophthalic acid and bipyridyl-type ligands

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Table S1 Selected geometric parameters (Å, °) for (**1**)

Complex (**1**)			
Zn1—O3^{i}	1.925 (2)	Zn1—N3^{ii}	2.024 (3)
Zn1—O1	1.974 (2)	Zn1—N2	2.037 (3)
O3^{i}—Zn1—O1	114.68 (10)	O3^{i}—Zn1—N2	113.85 (11)
O3^{i}—Zn1—N3^{ii}	114.41 (11)	O1—Zn1—N2	97.80 (11)
O1—Zn1—N3^{ii}	105.85 (11)	N3^{ii}—Zn1—N2	108.74 (12)

Symmetry codes: (i) −x+3/2, y−1/2, −z+1/2; (ii) x−1/2, −y+1/2, z−1/2.

Table S2 Hydrogen-bond geometry (Å, º) for (**1**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11···O4^{iii}	0.871 (10)	2.38 (3)	3.050 (4)	134 (3)
C25—H25B···Br3^{iv}	0.96	2.81	3.513 (12)	131.2
C25—H25A···O2^{v}	0.96	2.53	3.486 (11)	174.4
C12—H12A···O4^{vi}	0.93	2.59	3.373 (4)	142.4
C13—H13···O4^{i}	0.93	2.47	3.266 (4)	143.9

Symmetry codes: (i) −x+3/2, y−1/2, −z+1/2; (iii) x−1, y, z; (iv) x−1/2, −y+3/2, z+1/2; (v) −x+1/2, y+1/2, −z+1/2; (vi) x−1/2, −y+1/2, z+1/2.

Table S3 Halogen-bond geometry (Å, º) for (**1**)

C-Br···Br-C	*C-Br*	*Br···Br*	*Br-C*	*C-Br···Br-C*
C7-Br2···Br1^{vii}-C3	1.8949 (34)	3.5478 (5)	1.9017 (28)	137.087 (106)

Symmetry codes: (vii) -1+*x*, *y*, *z*.

Table S4 Selected geometric parameters (Å, °) for (**2**)

Complex (**2**)			
O4—Zn1^{i}	2.070 (5)	O1—Zn1	2.024 (4)
N1—Zn1	2.157 (5)	O1W—Zn1	2.262 (5)

N5—Zn1	2.226 (6)	Zn1—O2W	2.139 (5)
O1—Zn1—O4^{ii}	99.63 (19)	O2W—Zn1—N5	93.0 (2)
O1—Zn1—O2W	171.3 (2)	N1—Zn1—N5	172.1 (2)
O4^{ii}—Zn1—O2W	88.9 (2)	O1—Zn1—O1W	94.5 (2)
O1—Zn1—N1	87.84 (19)	O4^{ii}—Zn1—O1W	164.67 (18)
O4^{ii}—Zn1—N1	98.4 (2)	O2W—Zn1—O1W	77.2 (2)
O2W—Zn1—N1	89.3 (2)	N1—Zn1—O1W	88.0 (2)
O1—Zn1—N5	88.7 (2)	N5—Zn1—O1W	85.2 (2)
O4^{ii}—Zn1—N5	89.2 (2)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.

Table S5 Hydrogen-bond geometry (Å, °) for (**2**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*W*—H3*WB*···O3^{i}	0.85	1.95	2.790 (7)	171
O2*W*—H2*WA*···O3^{ii}	0.85	1.99	2.609 (8)	129
O2*W*—H2*WB*···O3*W*^{iii}	0.85	2.13	2.914 (7)	153
O1*W*—H1*WB*···O3*W*^{iii}	1.00	2.09	2.866 (6)	133
N2—H2···O2^{iii}	0.86	2.11	2.857 (8)	144
N3—H3···O6^{iv}	0.86	2.43	3.161 (8)	144
N4—H4*A*···O2*W*^{v}	0.86	2.54	3.204 (9)	135
O1*W*—H1*WA*···O5^{v}	0.96	1.77	2.706 (8)	163
C21—H21···N3^{vi}	0.93	2.59	2.900 (10)	100
O2*W*—H2*WA*···Br3^{vi}	0.85	2.61	3.314 (5)	141
O3*W*—H3*WA*···O6^{vi}	0.85	2.17	2.963 (8)	154

Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) *x*+1, *y*, *z*; (iv) *x*−1/2, −*y*+3/2, −*z*; (v) −*x*+2, *y*−1/2, −*z*+1/2; (vi) −*x*+3/2, −*y*+1, *z*+1/2.

Table S6 Halogen-bond geometry (Å, º) for (**2**)

C-Br···Br-C	*C-Br*	*Br···Br*	*Br-C*	*C-Br···Br-C*

C3-Br2···Br1^{vii}-C7	1.9013 (63)	3.487 (1)	1.9016 (71)	142.648 (187)

Symmetry codes: (vii) -1+*x*, *y*, *z*.

Table S7 Halogen-bond geometry (Å, º) for (**2**)

C-O···Br	*C-O*	*O···Br*	*C···Br*	*C-O···Br*
C8-O3···Br3^{viii}	1.258 (4)	3.2347 (47)	3.0875 (70)	151.207 (422)

Symmetry codes: (viii) *x*-1/2, -*y*+1/2, -*z*.

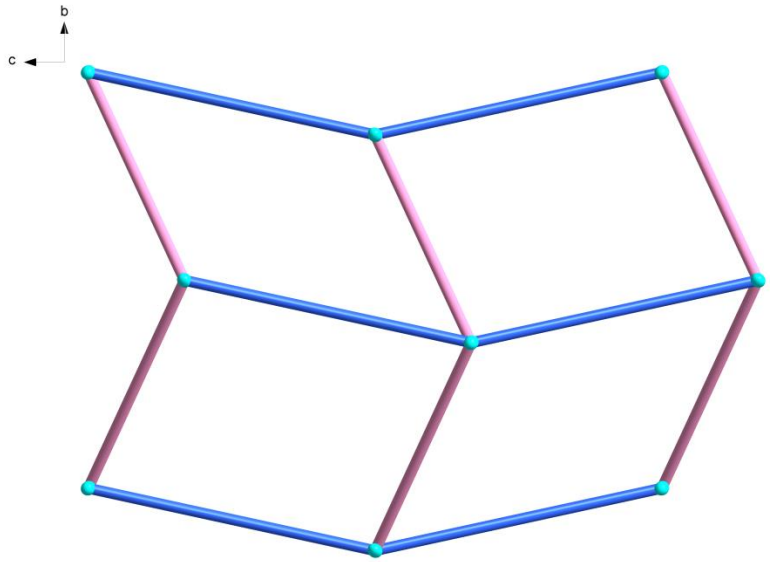


Figure S1 Simplified representation of the 2D (4, 4) topological network of (**1**).

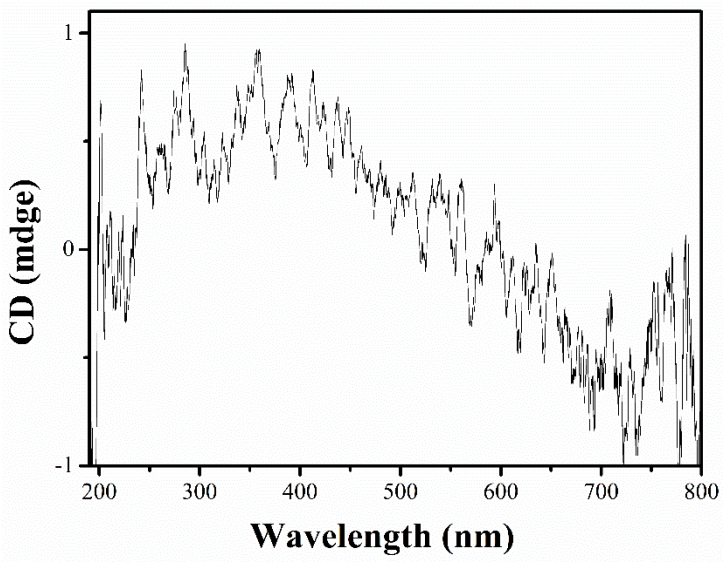
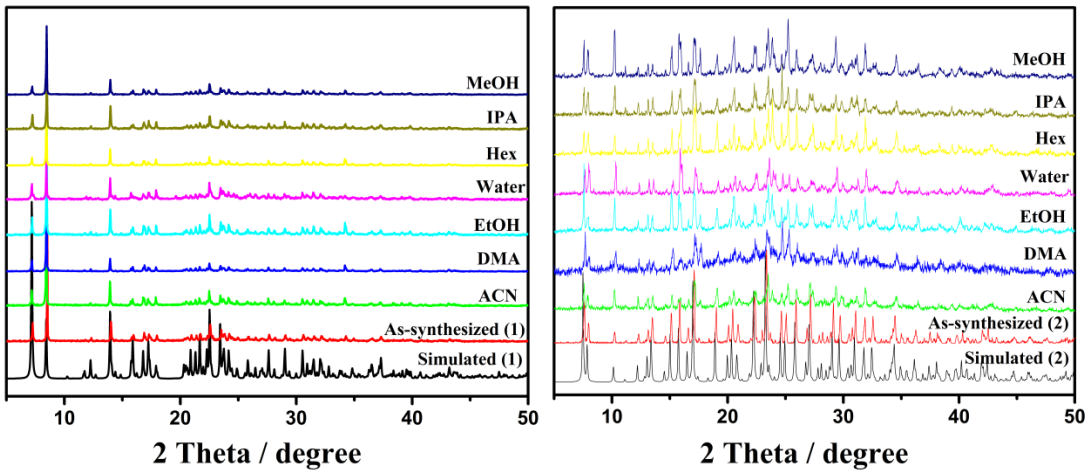
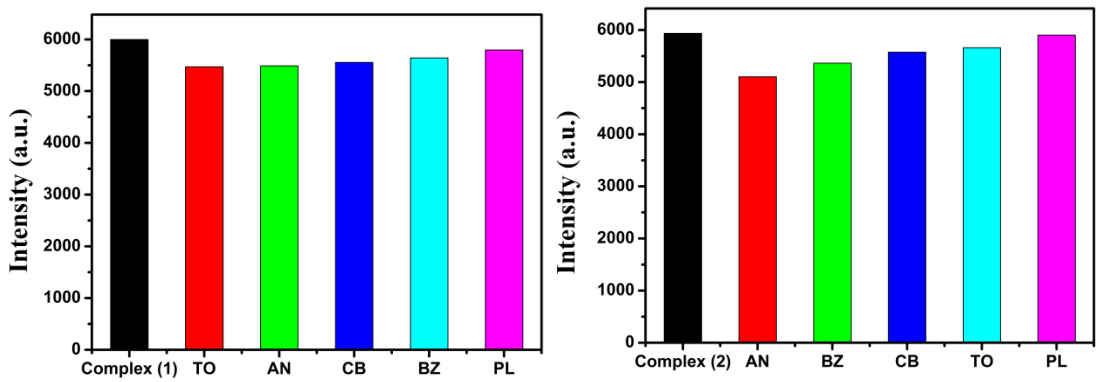


Figure S2 CD spectrum of complex (**2**) in KBr pellet.



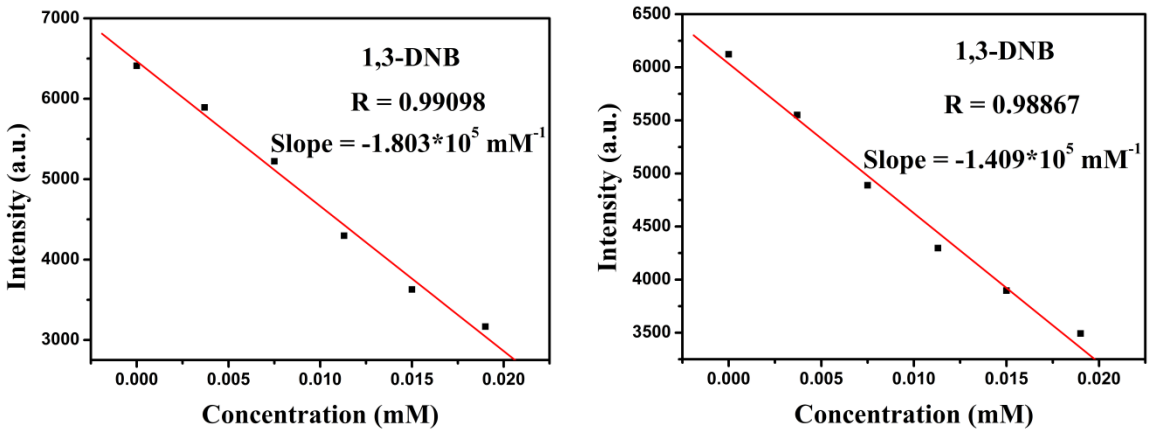
(**A**) (**B**)

Figure S3 The PXRD patterns of (**1**) (**A**) and (**2**) (**B**) after soaking in different solvents.



(**A**) (**B**)

Figure S4 The maximum fluorescence intensity of the methanol suspensions of (**1**) (**A**) and (**2**) (**B**) containing each 0.075 mmol/L electron-rich aromatic compounds.



(**A**)

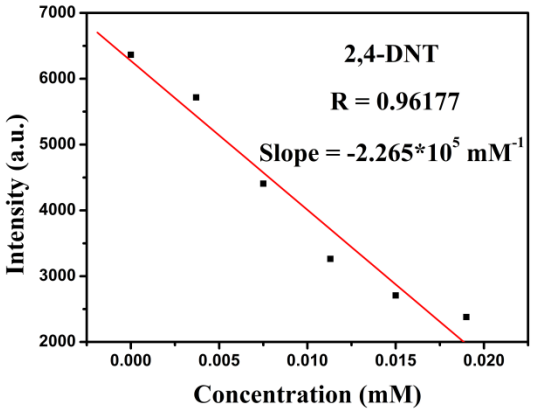
$m = 1.803 \times 10^5\ mM^{-1}$

(**H**)

$m = 1.409 \times 10^5\ mM^{-1}$

δ = 149.89 (N = 7)

3δ/m = 3.649 × 10^{-3} mM

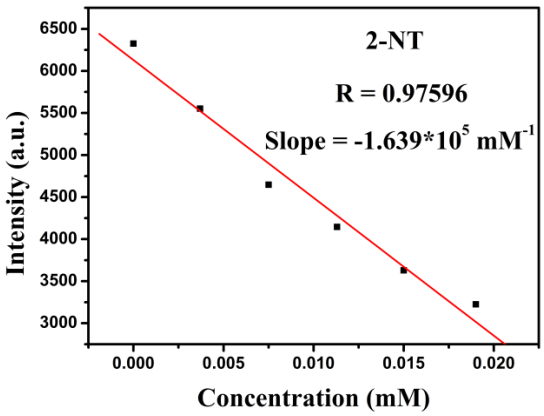


(**B**)

m = 2.265 × 10^{5} mM^{-1}

δ = 149.89 (N = 7)

3δ/m = 1.985 × 10^{-3} mM



(**C**)

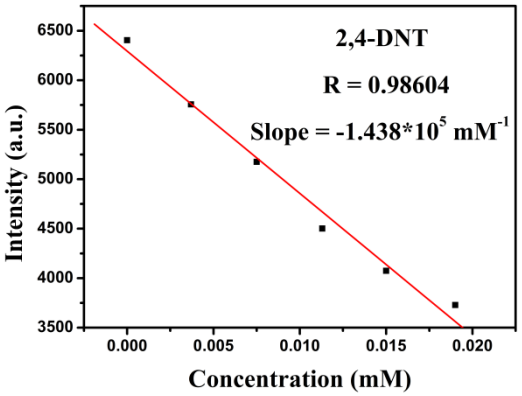
m = 1.639 × 10^{5} mM^{-1}

δ = 149.89 (N = 7)

3δ/m = 2.744 × 10^{-3} mM

δ = 219.28 (N = 7)

3δ/m = 4.669 × 10^{-3} mM

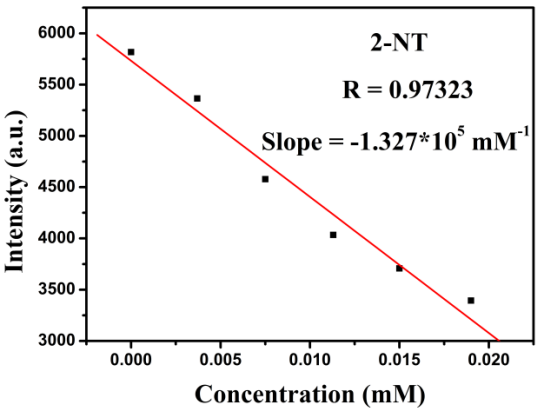


(**I**)

m = 1.438 × 10^{5} mM^{-1}

δ = 219.28 (N = 7)

3δ/m = 4.575 × 10^{-3} mM

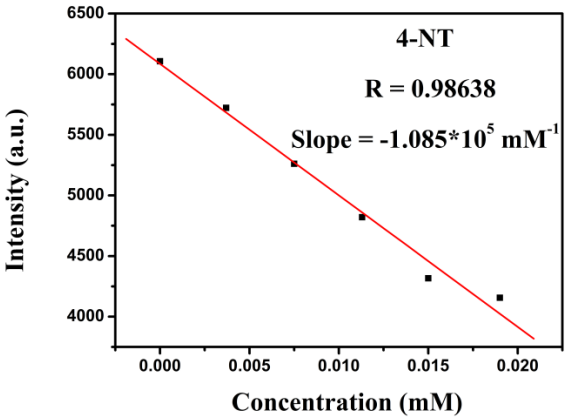


(**J**)

m = 1.327 × 10^{5} mM^{-1}

δ = 219.28 (N = 7)

3δ/m = 4.957 × 10^{-3} mM

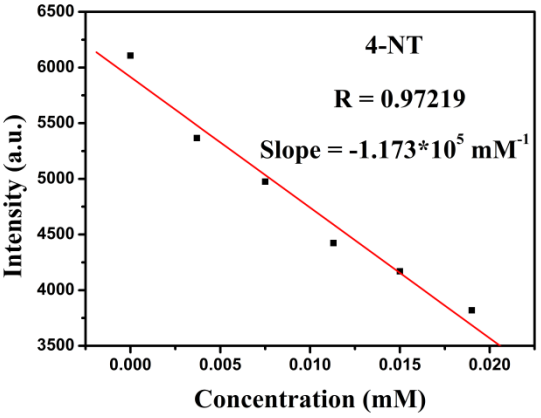


(D)

m = 1.259 × 10 5 mM-1

δ = 149.89 (N = 7)

3δ/m = 3.572 × 10-3 mM

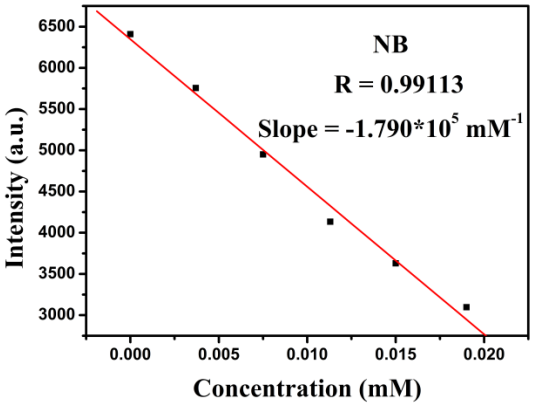


(K)

m = 1.173 × 10 5 mM-1

δ = 219.28 (N = 7)

3δ/m = 5.608 × 10 -3 mM

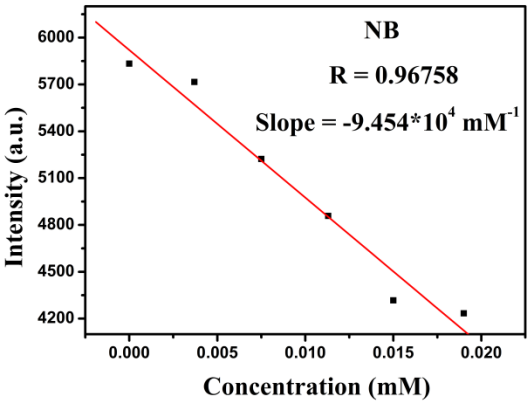


(E)

m = 1.790 × 10 5 mM-1

δ = 149.89 (N = 7)

3δ/m = 2.512 × 10-3 mM

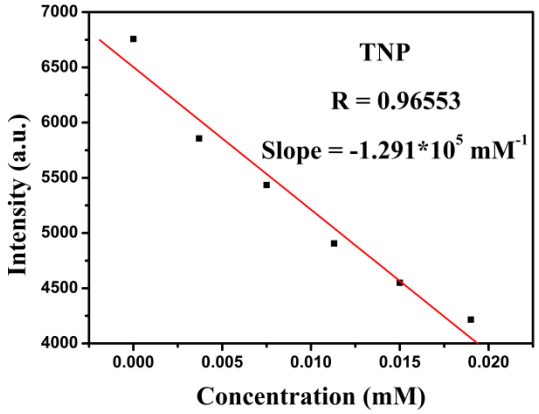


(L)

m = 9.454 × 10 4 mM-1

δ = 219.28 (N = 7)

3δ/m = 6.958 × 10 -3 mM

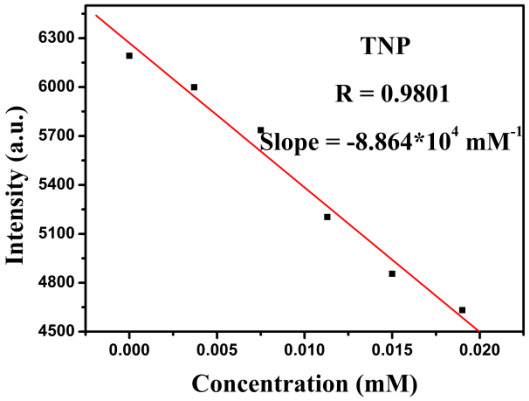


(F)

m = 1.291 × 10^{5} mM^{-1}

δ = 149.89 (N = 7)

3δ/m = 3.483 × 10^{-3} mM

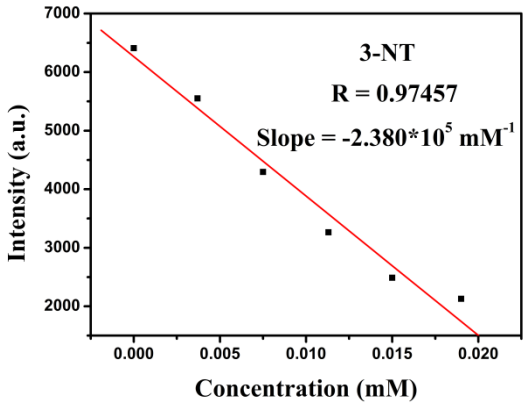


(M)

m = 8.864 × 10^{4} mM^{-1}

δ = 219.28 (N = 7)

3δ/m = 7.421 × 10^{-3} mM

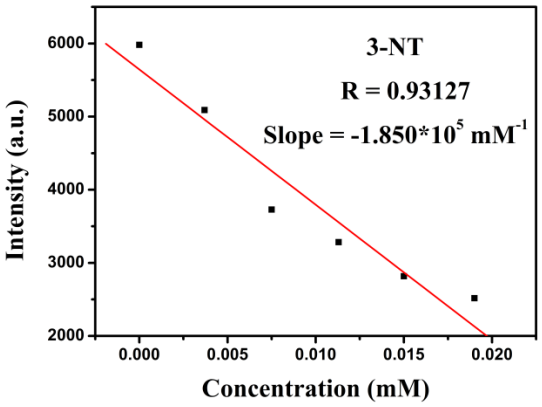


(G)

m = 2.380 × 10^{5} mM^{-1}

δ = 149.89 (N = 7)

3δ/m = 1.889 × 10^{-3} mM



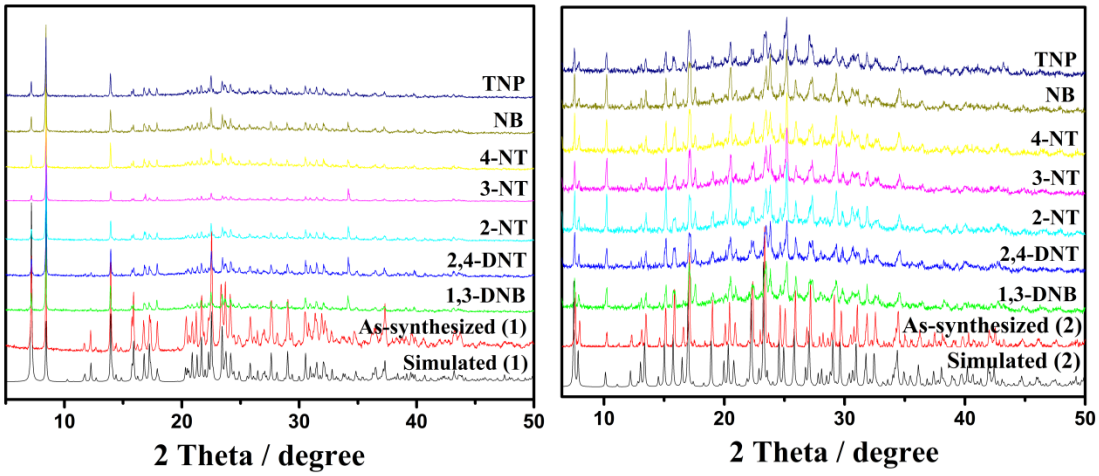
(N)

m = 1.850 × 10^{5} mM^{-1}

δ = 219.28 (N = 7)

3δ/m = 3.556 × 10^{-3} mM

Figure S5 The best linear fitting of the fluorescence intensity of the methanol suspensions of (**1**) (**A-G**) and (**2**) (**H-N**) *versus* the NAEs concentration of 0 - 0.01875 mmol/L.



(**A**) (**B**)

Figure S6 The PXRD patterns of the samples after soaking (**1**) (**A**) and (**2**) (**B**) in different methanol solutions of NAEs (0.075 mol/L).