

Electronic Supplementary Information

Aqueous phase selective 2,4,6-trinitrophenol detection via fluorescent metal-organic framework with pendant recognition site

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Figures:-

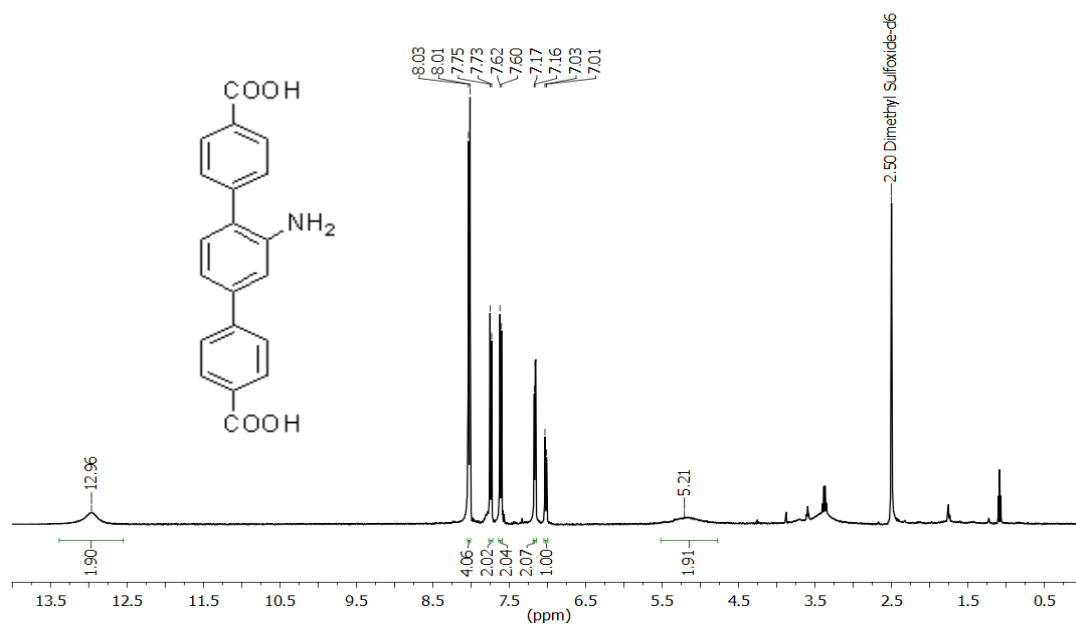


Figure S1: ^1H NMR of ligand L in DMSO- d_6 .

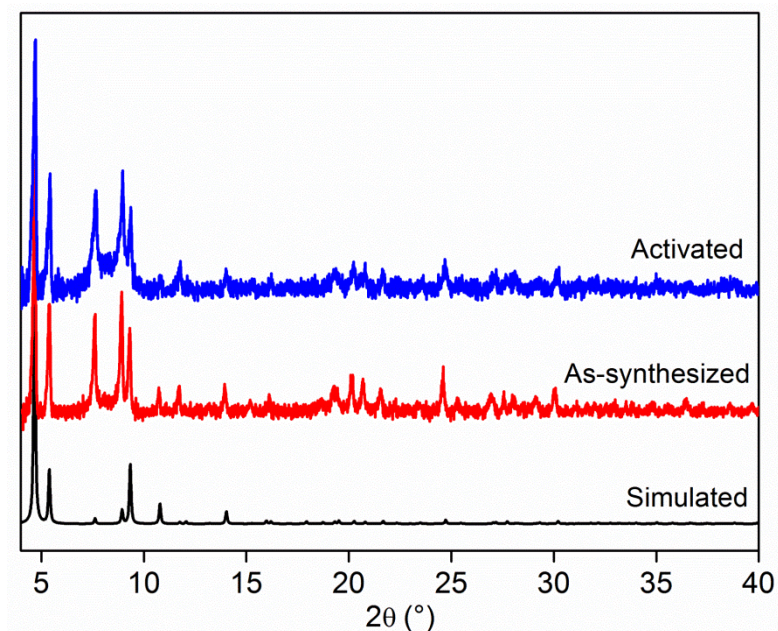


Figure S2: Powder X-ray diffraction patterns (PXRD) of simulated, as-synthesized and activated MOF 1.

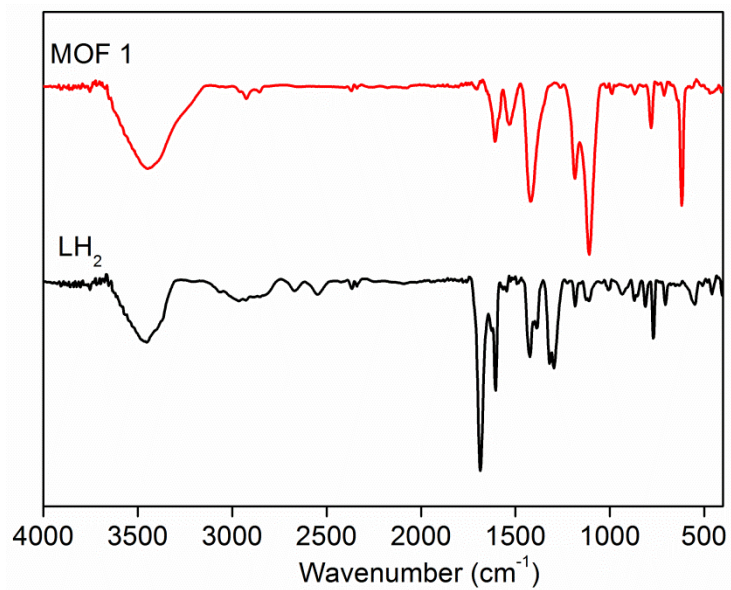


Figure S3: FT-IR spectra of Ligand LH₂ and MOF 1.

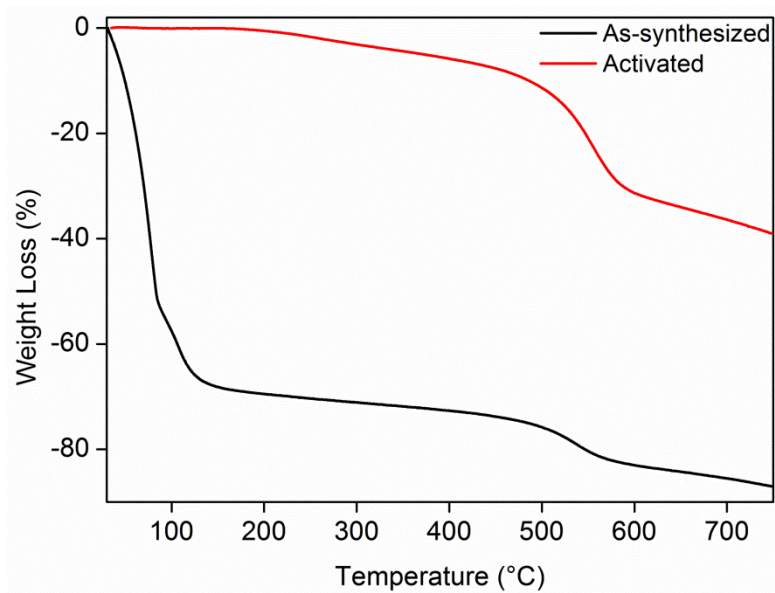


Figure S4: Thermogravimetric analysis of as-synthesized and activated MOF 1.

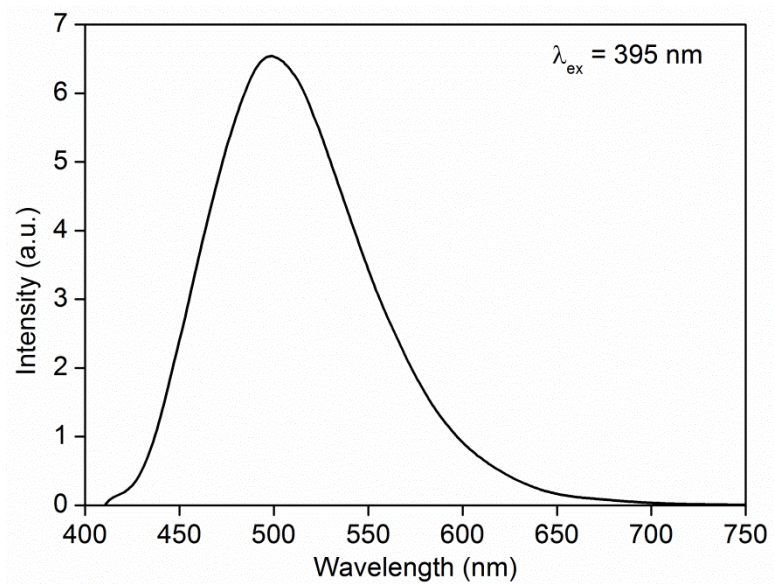


Figure S5: Emission spectra of MOF (**1'**) dispersed in water upon excitation at 395 nm.

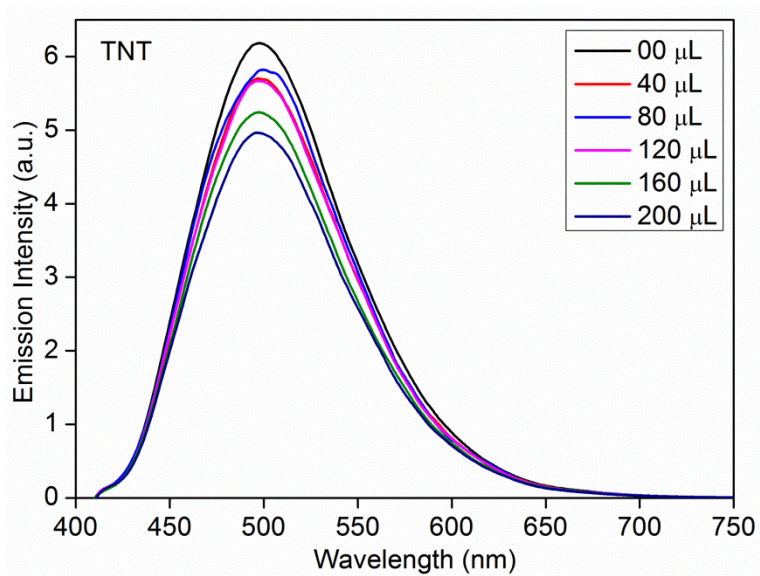


Figure S6: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of TNT solution (1mM) in water.

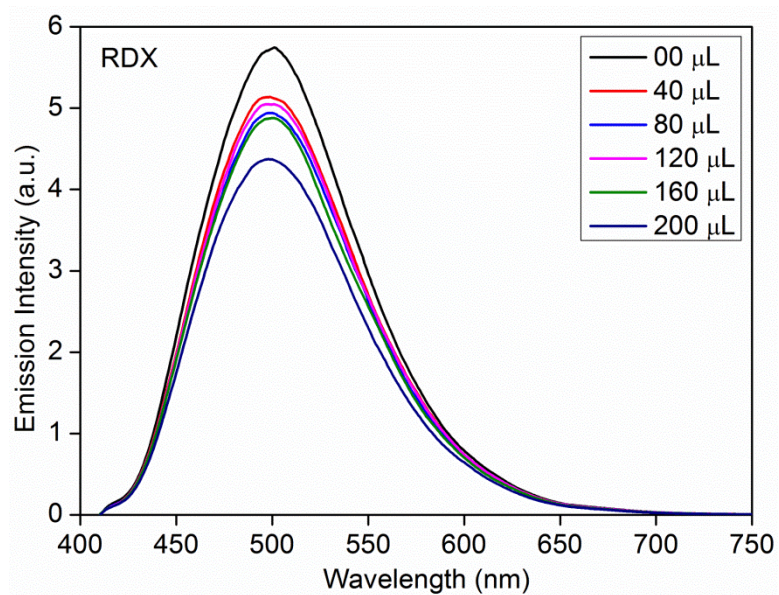


Figure S7: Emission spectra of MOF (1') dispersed in water upon incremental addition of RDX solution (1mM) in water.

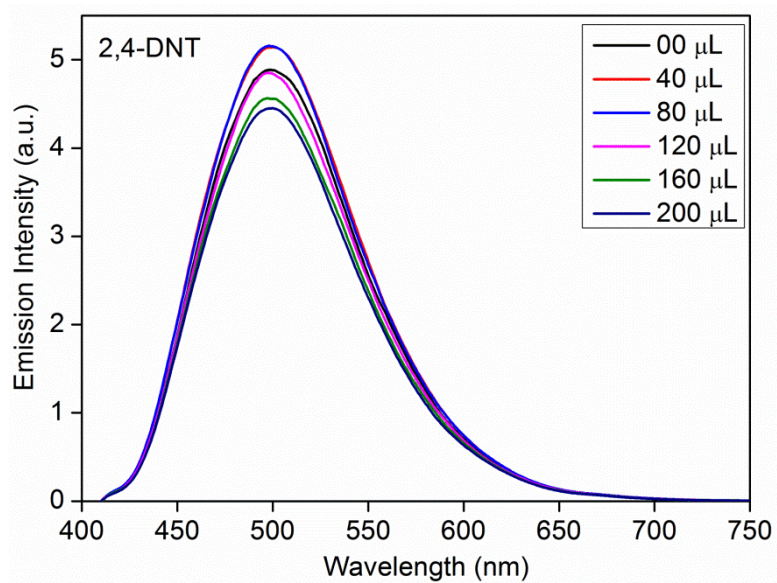


Figure S8: Emission spectra of MOF (1') dispersed in water upon incremental addition of 2,4-DNT solution (1mM) in water.

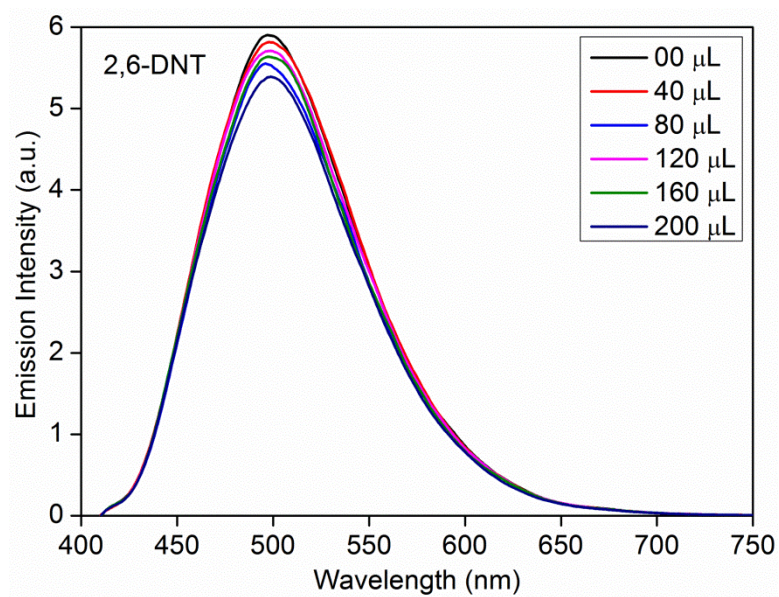


Figure S9: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of 2,6-DNT solution (1mM) in water.

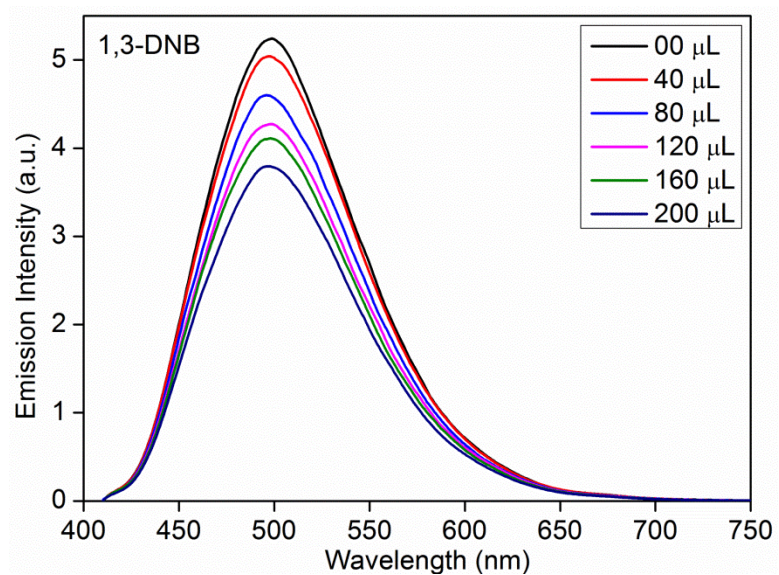


Figure S10: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of 1,3-DNB solution (1mM) in water.

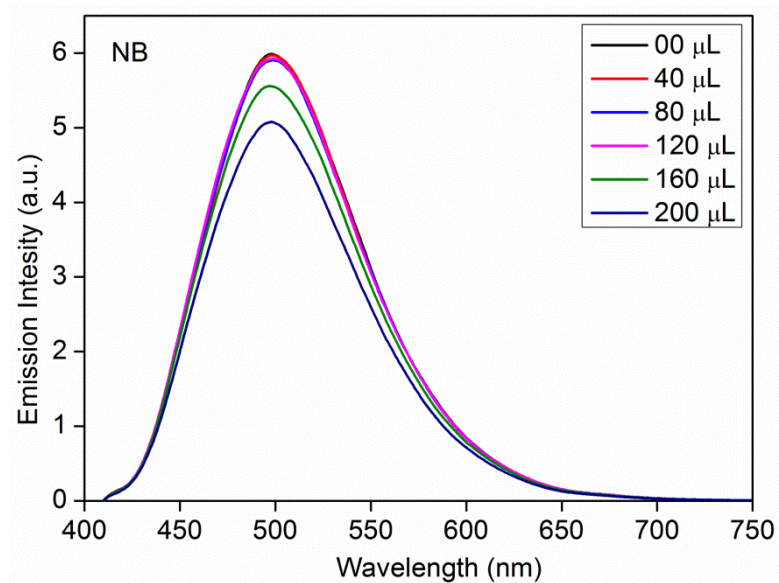


Figure S11: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of NB solution (1mM) in water.

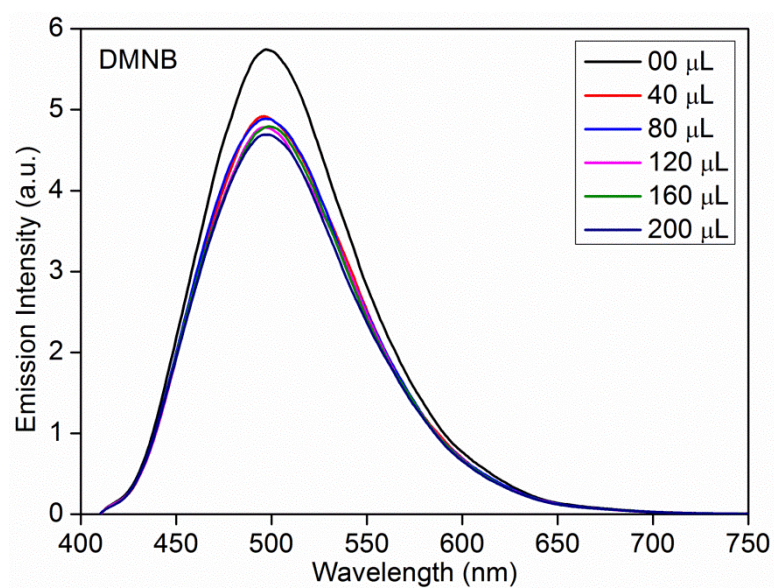


Figure S12: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of DMNB solution (1mM) in water.

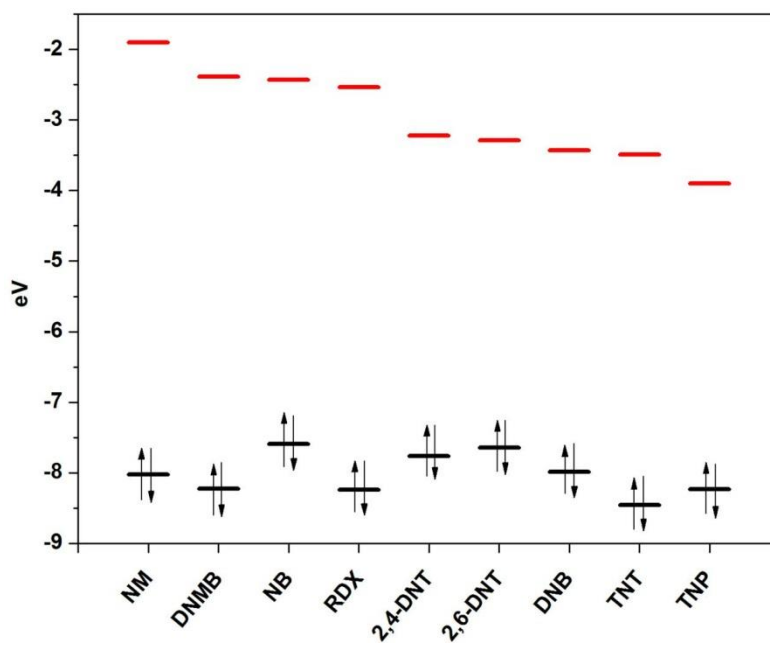


Figure S13: HOMO and LUMO energies of electron deficient nitro explosives (at B3LYP/6-31G* level of theory).²

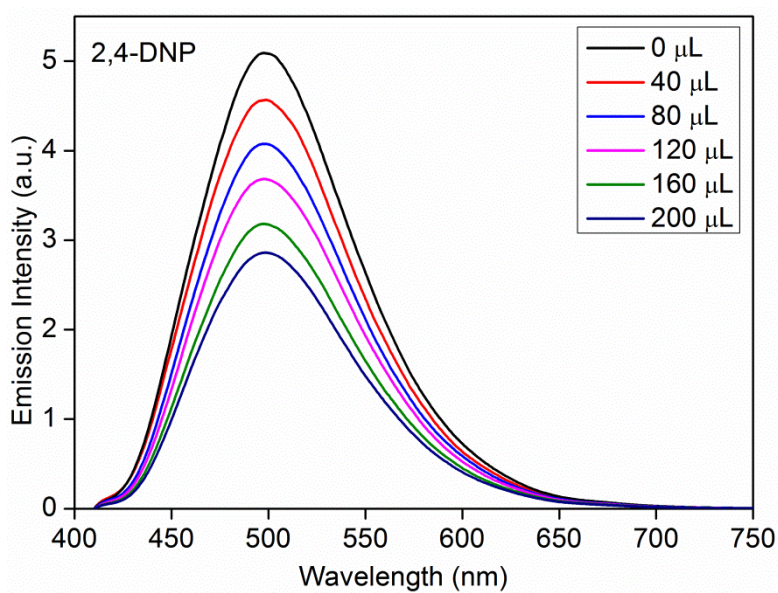


Figure S14: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of 2,4-DNP solution (1mM) in water.

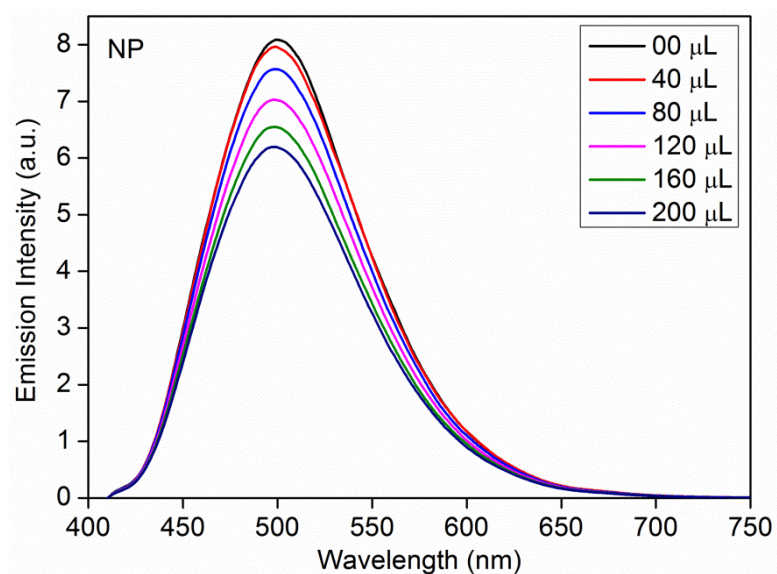


Figure S15: Emission spectra of MOF (**1'**) dispersed in water upon incremental addition of NP solution (1mM) in water.

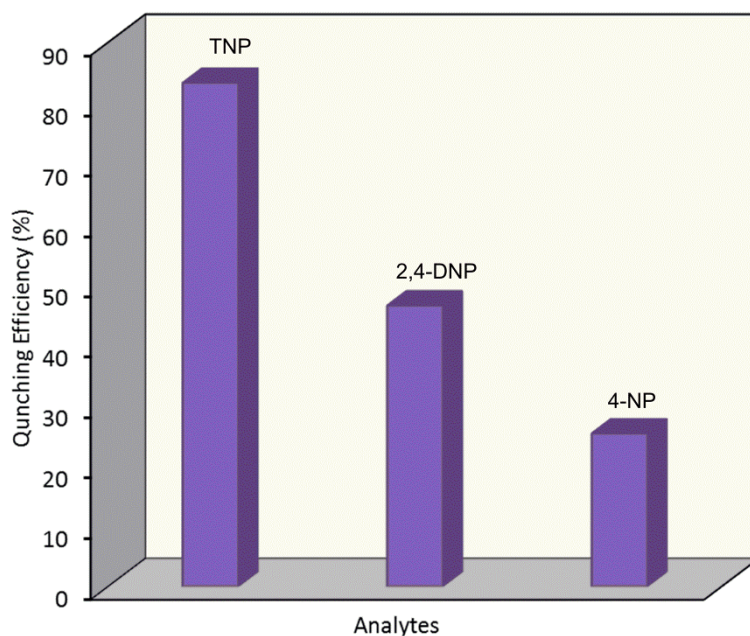


Figure S16: Comparison of percentage fluorescence quenching obtained upon addition of TNP, 2,4-DNP, NP to **1'** dispersed in water.

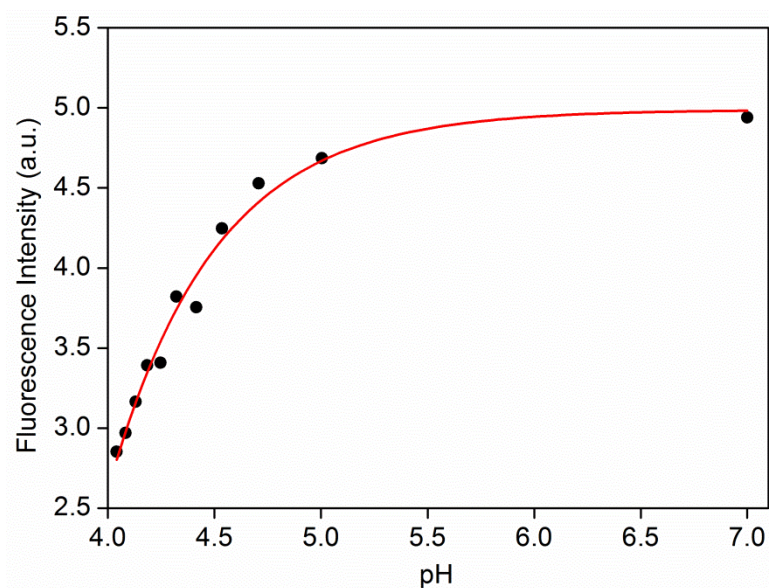


Figure S17: Effect of pH on fluorescence intensity of MOF 1'.

Table:

Table S1:- Approximate sizes of explosive analytes.²

No.	Analytes	Approximate Size (D × W × L, Å)
1	TNT	5.6 X 7.7 X 10.2
2	RDX	5.8 X 6.3 X 8.8
3	TNP	5.0 X 6.2 X 7.1
4	2,6 DNT	5.6 X 7.7 X 9.5
5	2,4 DNT	5.6 X 7.7 X 10.1
6	1,3 DNB	5.0 X 7.7 X 8.6
7	NB	3.4 X 6.2 X 8.6
8	DMNB	7.1 X 7.3 X 7.7

References:

- 1) A. Schaate, P. Roy, A. Godt, J. Lippke, F. Waltz, M. Wiebcke and P. Behrens, *Chem. Eur. J.*, 2011, **17**, 6643.
- 2) S. S. Nagarkar, B. Joarder, A. K. Chaudhari, S. Mukherjee and S. K. Ghosh, *Angew. Chem., Int. Ed.*, 2013, **52**, 2881.