

Electronic Supporting Information

Selective luminescent sensing of metal ions and nitro-aromatics over a porous mixed-linker cadmium(II) based metal-organic framework

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Table S1. Bond distances (Å) and angles (°) around the metal centre in Cd-MOF1

Atoms	Distance	Atoms	Distance
Cd1 - O1	2.241(5)	Cd1 - O4 ^a	2.437(6)
Cd1 - O3 ^a	2.325(6)	Cd1 - N3	2.368(6)
Cd1 - O2 ^b	2.324(6)		
Atoms	Angle	Atoms	Angle
O1 - Cd1 - N3	90.57(10)	O2 ^b - Cd1 - N3	86.68(11)
O1 - Cd1 - O3 ^a	142.72(18)	N3 - Cd1 - N3 ^c	172.32(15)
O1 - Cd1 - O4 ^a	88.27(18)	O3 ^a - Cd1 - O4 ^a	54.45(16)
O1 - Cd1 - O2 ^b	128.73(18)	O2 ^b - Cd2 - O3 ^a	88.56(15)
O3 ^a - Cd1 - N3	91.85(10)	O2 ^b - Cd2 - O4 ^a	143.01(15)
O4 ^a - Cd1 - N3	93.82(11)		
Symmetry element ^a = 1-x,-1/2+y,3/2-z; ^b = x,1-y,1-z; ^c = 1-x,y,z			

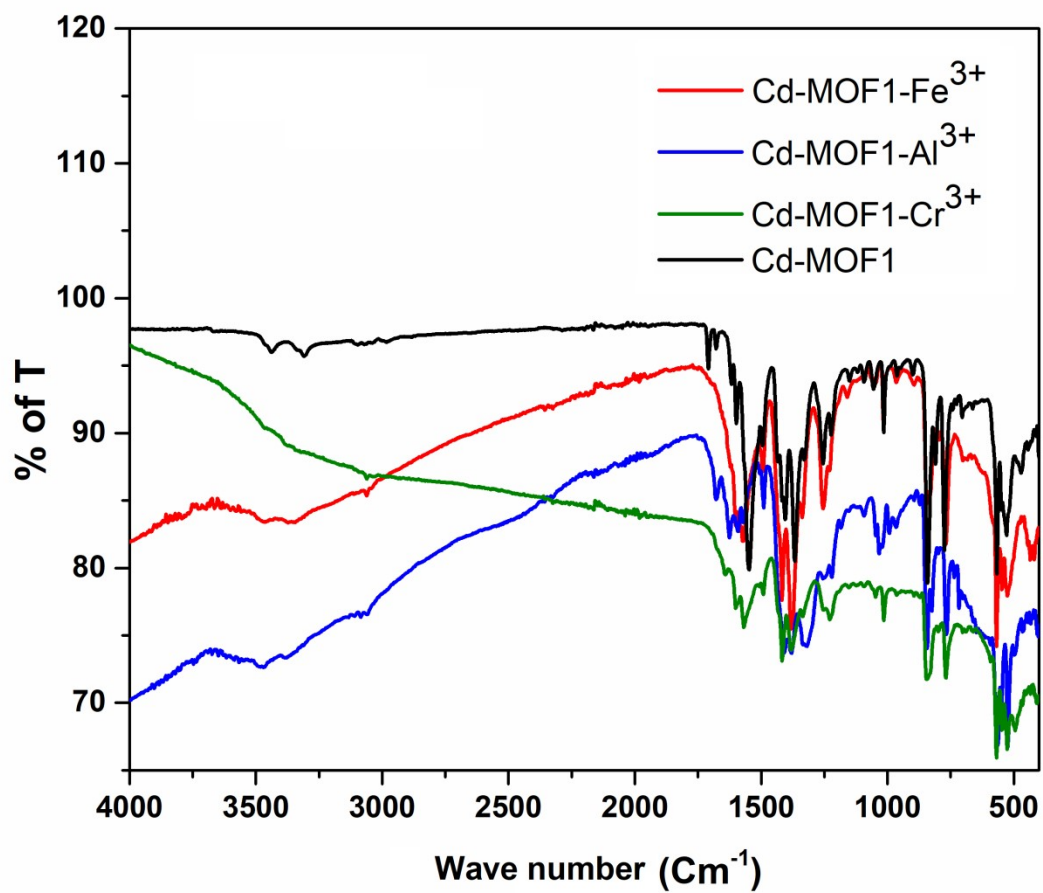


Fig. S1 IR spectra of Cd-MOF1 and Cd-MOF1 treated with various metal salt solutions

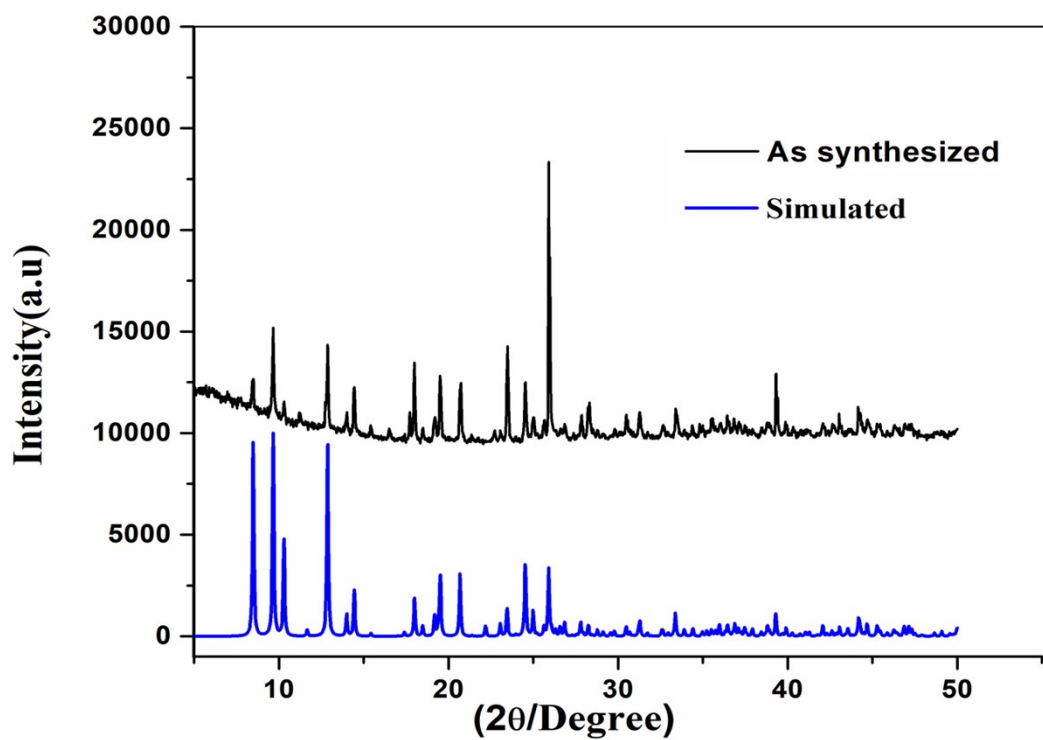


Fig. S2 Powder X-ray diffraction pattern of Cd-MOF1 simulate (blue) and as synthesise (black).

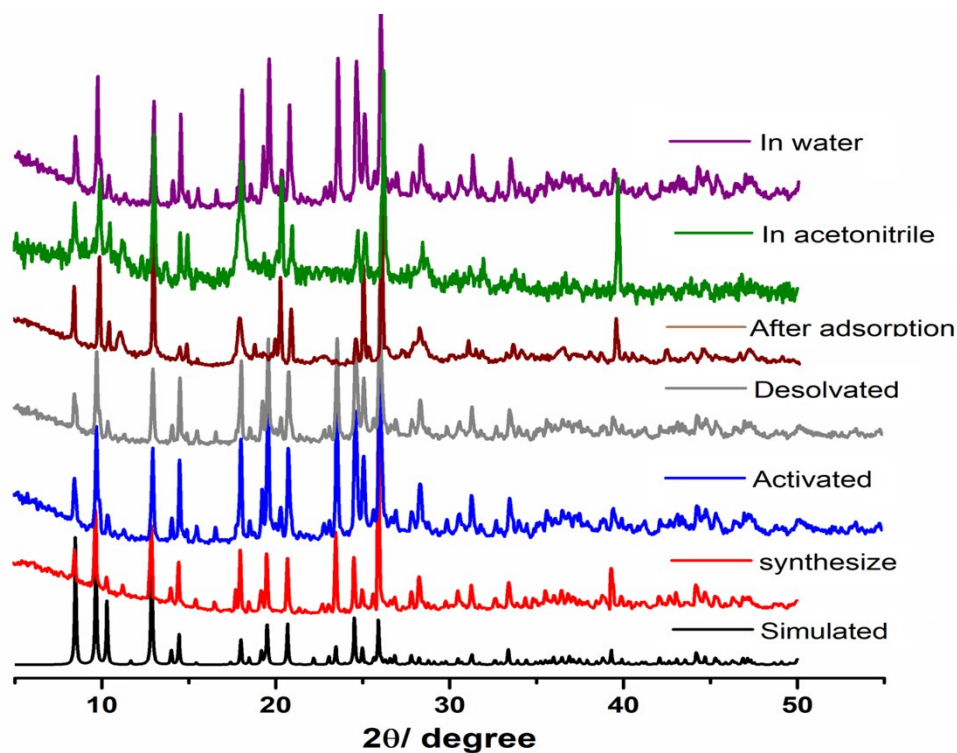


Fig. S3a Powder X-ray diffraction pattern of Cd-MOF1 at different conditions

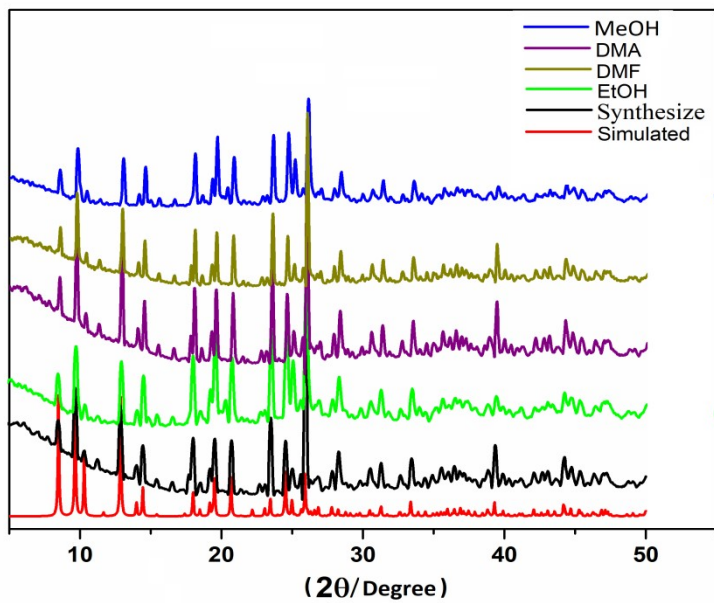


Fig. S3b Powder X-ray diffraction pattern of Cd-MOF1 after immersing in various solvents

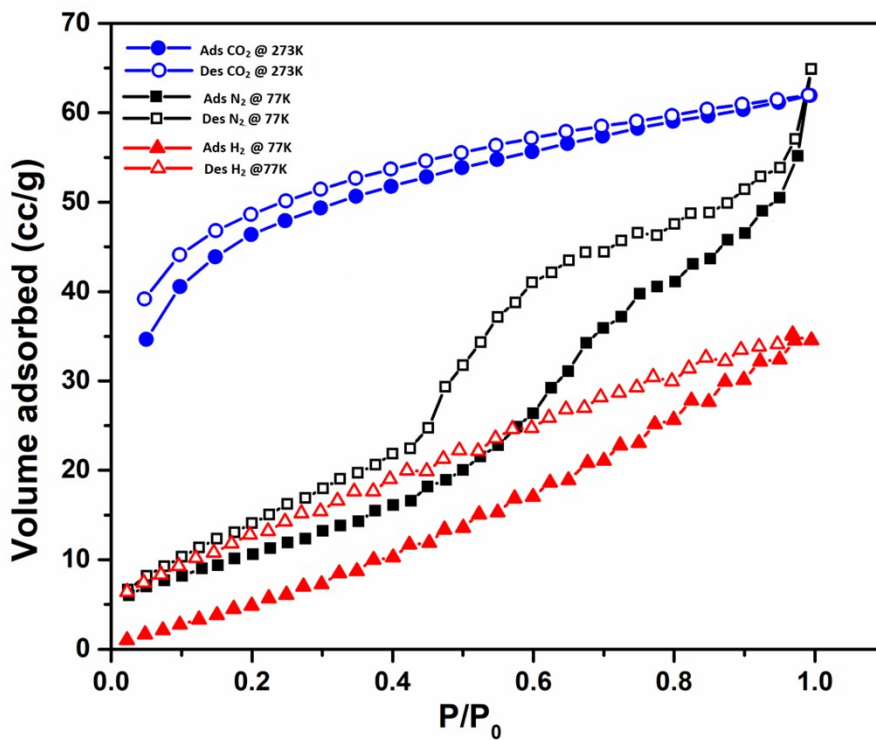


Fig. S4a Gas adsorption isotherms of N₂ (black), H₂ (red) measured at 77K and CO₂ (blue) measured at 273K

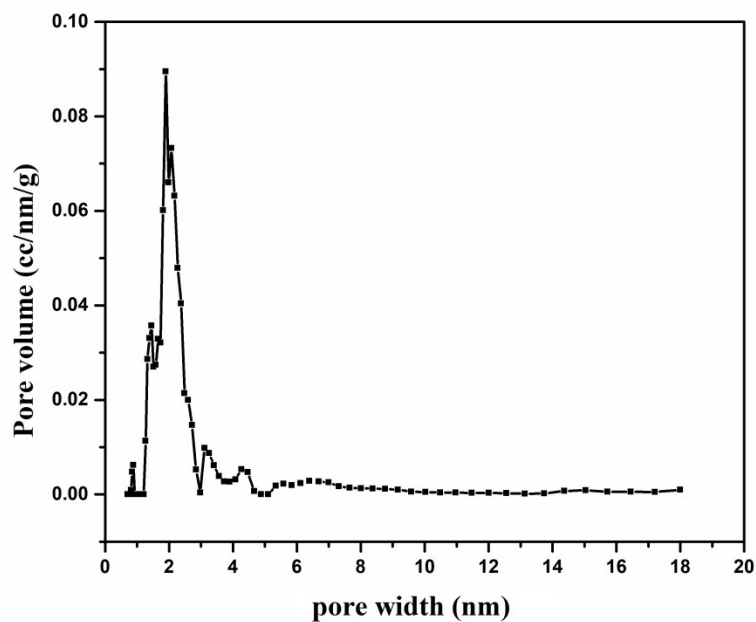


Fig. S4b Pore size distribution plot of Cd-MOF1 calculated using NLDFIT method

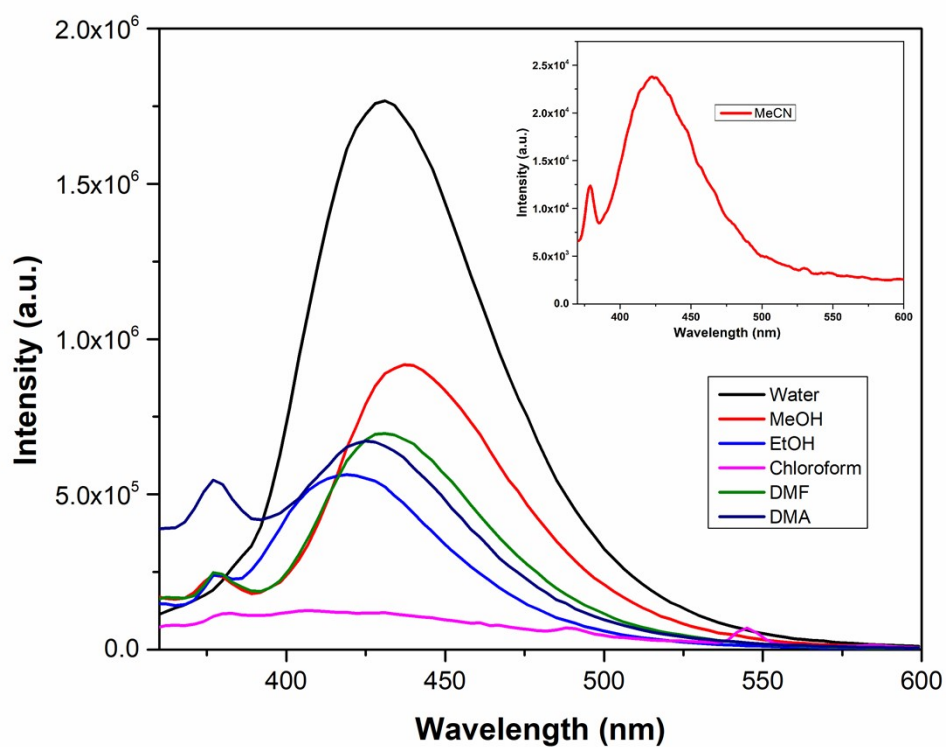


Fig. S5a Comparison of fluorescence spectra of Cd-MOF1 dispersed in various solvent media ($\lambda_{\text{ex}} = 370$ nm). Fluorescence response of Cd-MOF1 dispersed in MeCN (inset) is weaker than other solvents.

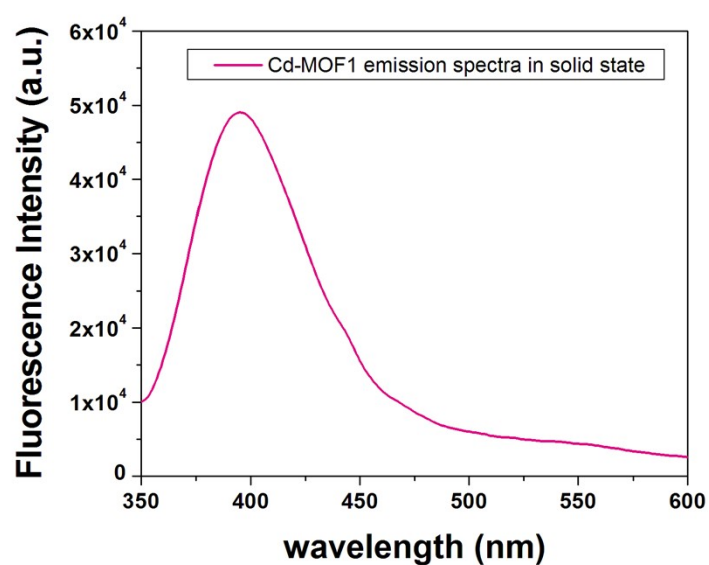


Fig. S5b Solid state emission spectrum of Cd-MOF1 ($\lambda_{\text{ex}} = 340$ nm).

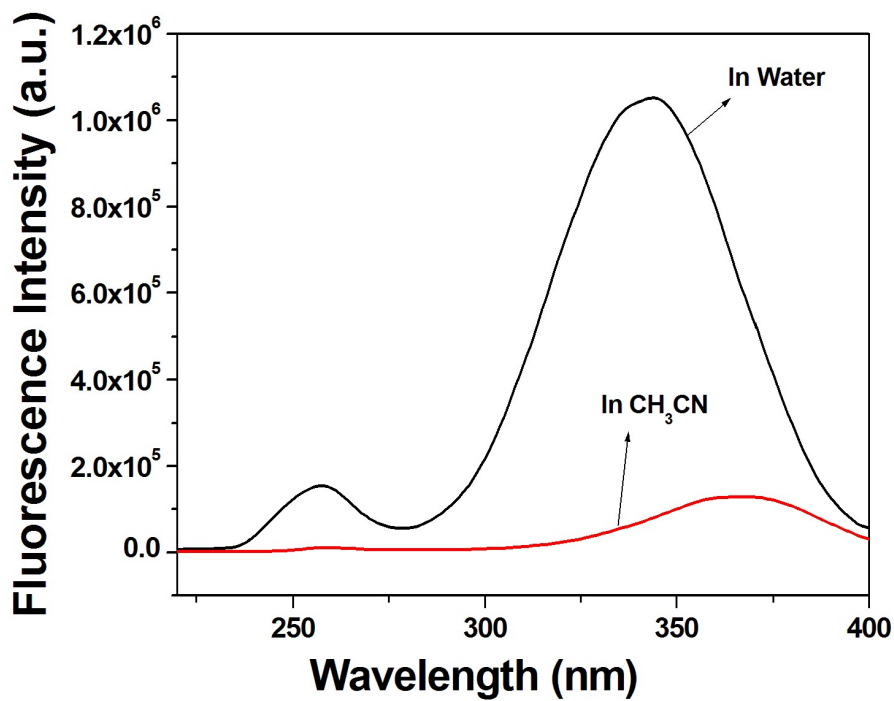


Fig. S5c Comparison of excitation spectrum of Cd-MOF1 (10 μ M) at $\lambda_{em} = 428$ nm in acetonitrile and water media.

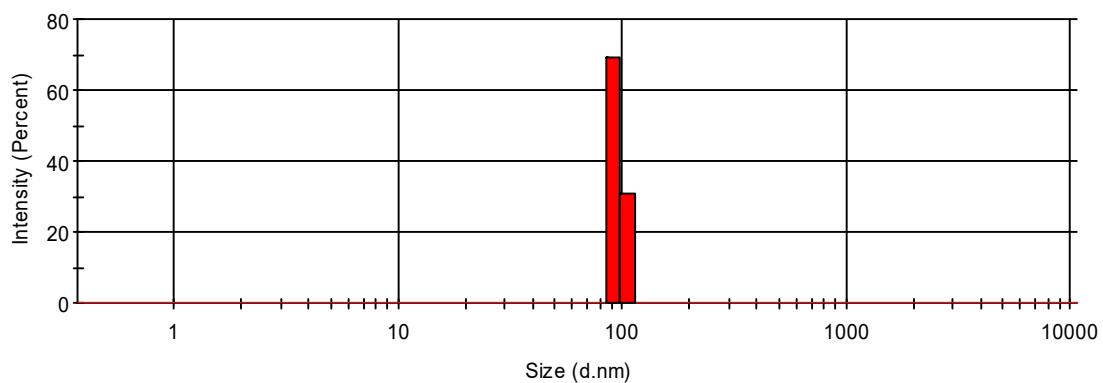


Fig. 6a Dynamic light scattering plot showing particle size distribution of Cd-MOF1 (2 μM) in water medium

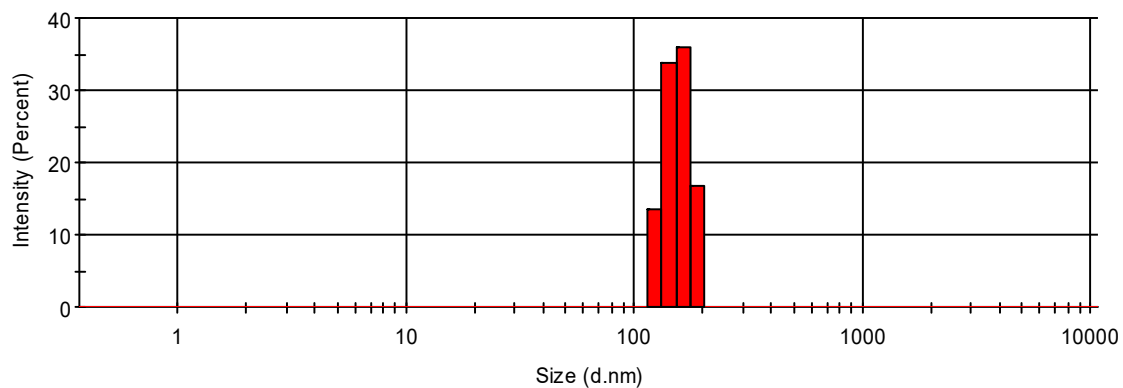


Fig. 6b Dynamic light scattering plot showing particle size distribution of Cd-MOF1 (2 μM) in presence of TNP (2 μM) in water medium

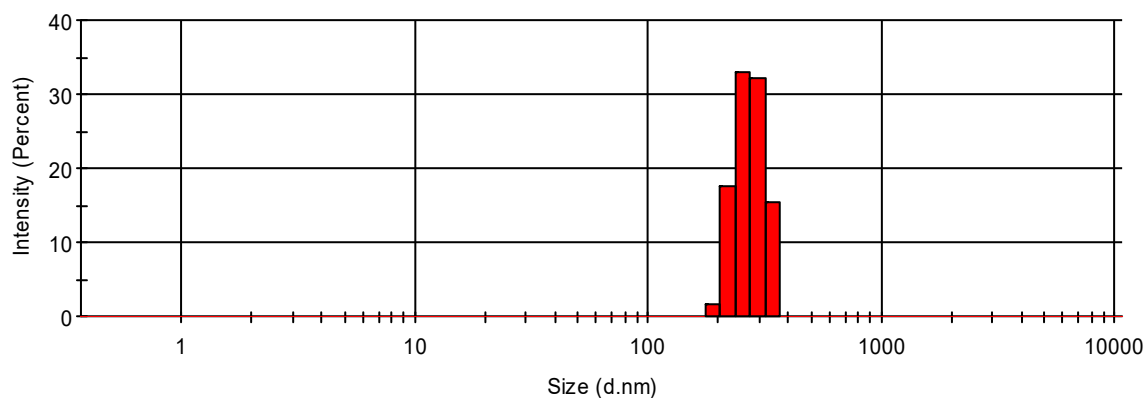


Fig 6c Dynamic light scattering plot showing particle size distribution of Cd-MOF1 (5 μM) in presence of TNP (5 μM) in water medium

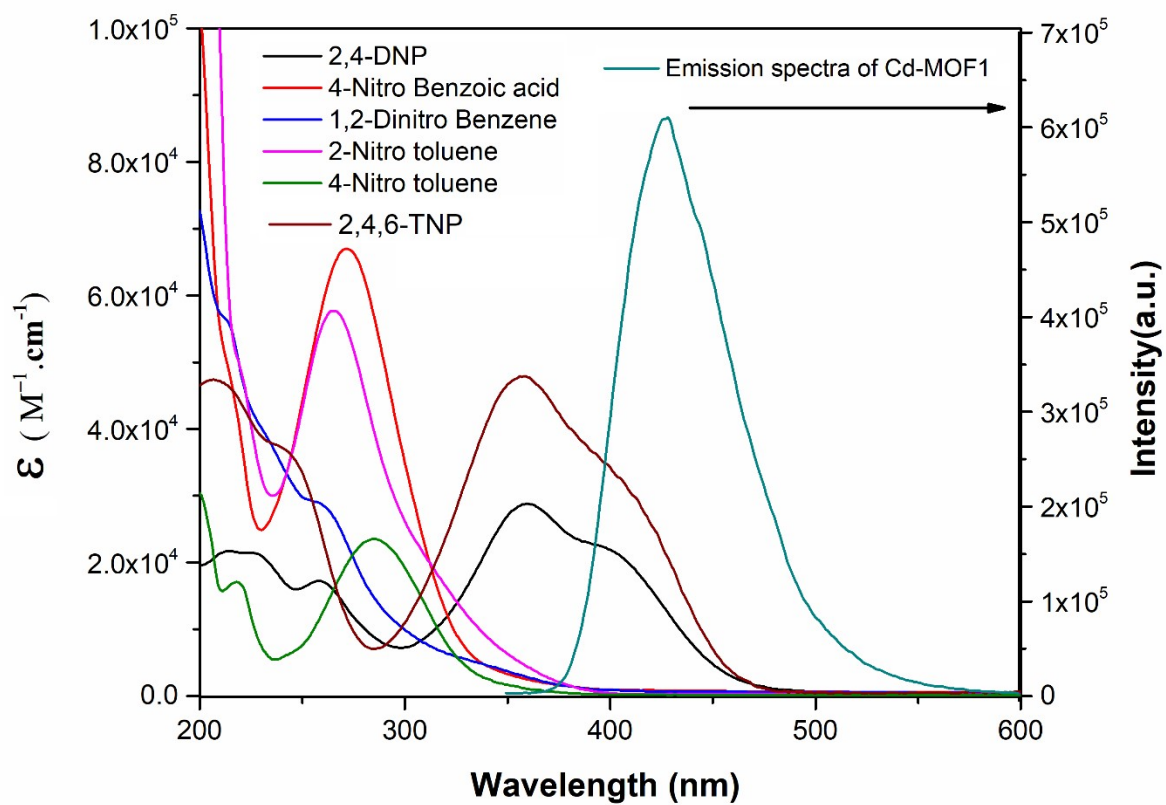


Fig. S7 Plot showing the extent of spectral overlap between absorption band of nitroaromatics and emission band of the Cd-MOF1

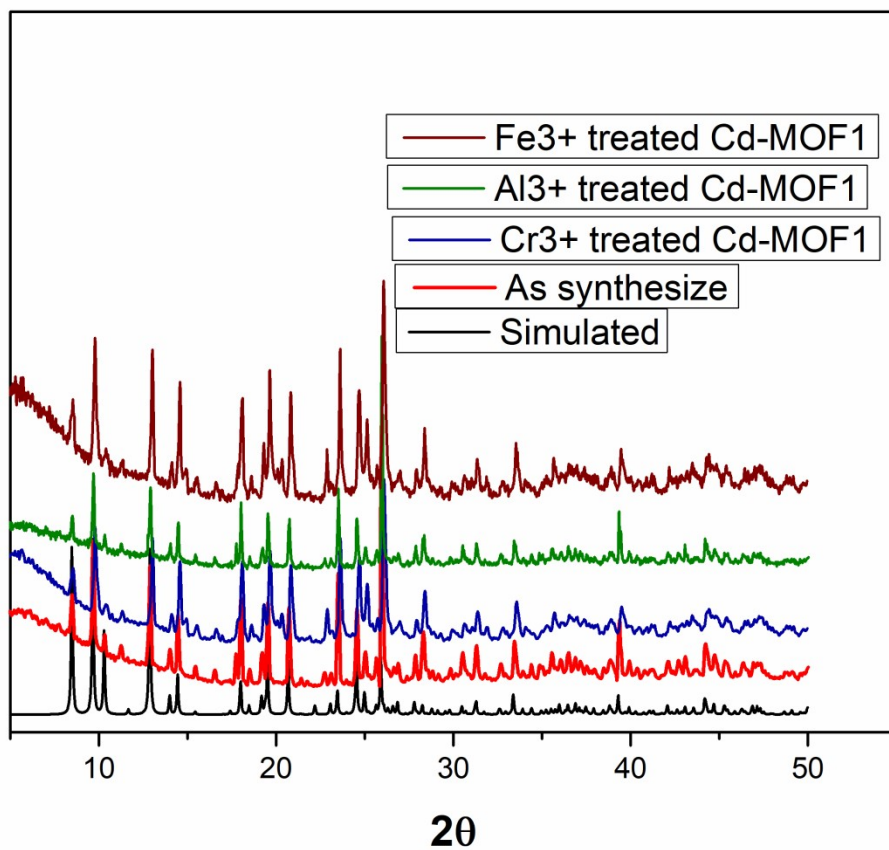
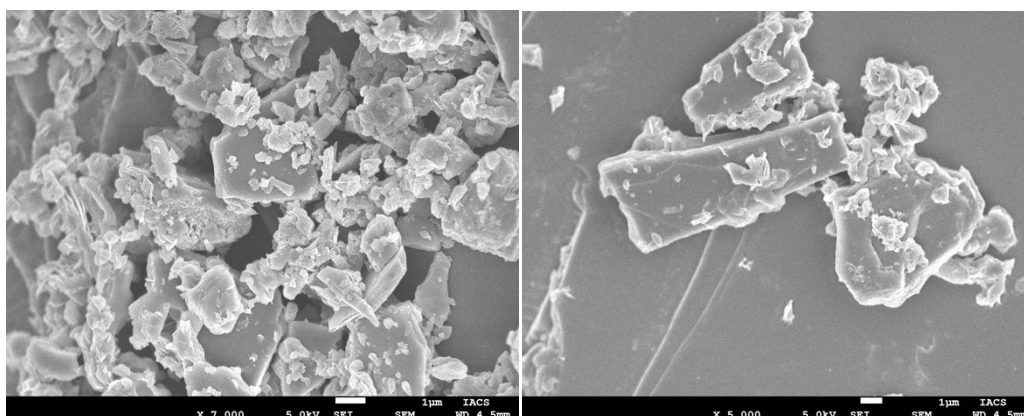


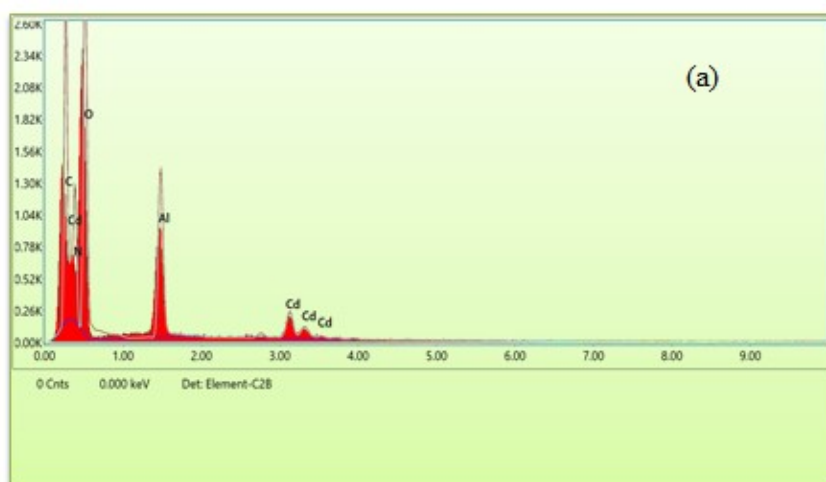
Fig. S8 Powder X-ray diffraction patterns of Cd-MOF1 and solid recovered after metal ion (Fe^{3+} , Al^{3+} and Cr^{3+}) sensing experiment



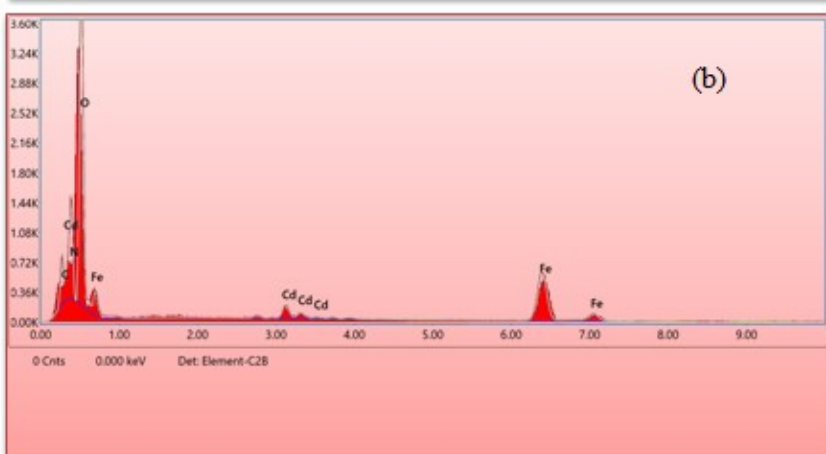
(A)

(B)

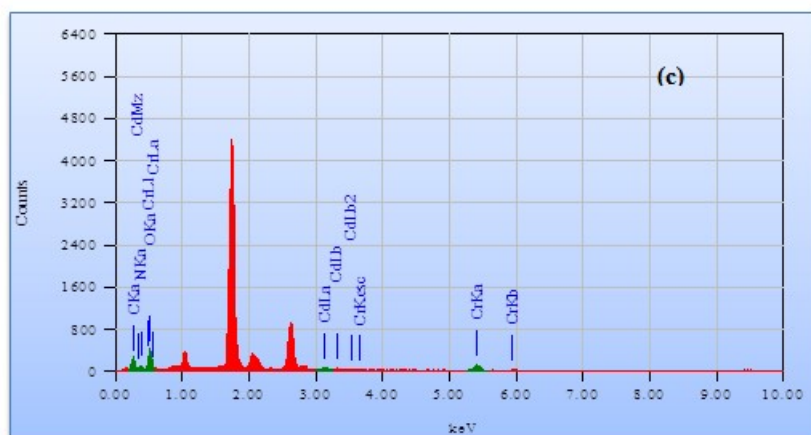
Fig. S9a FE-SEM images of pure Cd-MOF1 (A) and metal treated Cd-MOF1 (B)



Element	Weight %
C K	25.49
N K	16.89
O K	43.01
AlK	8.69
CdL	5.92



Element	Weight %
C K	7.16
N K	11.15
O K	39.99
CdL	4.68
FeK	37.02



Element	Weight %
C K	12.3528
N K	13.0594
O K	29.3898
CdL	14.3553
CrK	30.8427

Fig. S9b EDS analysis of (a) Al³⁺ treated Cd-MOF1; (b) Fe³⁺ treated Cd-MOF1; (c) Cr³⁺ treated Cd-MOF1.

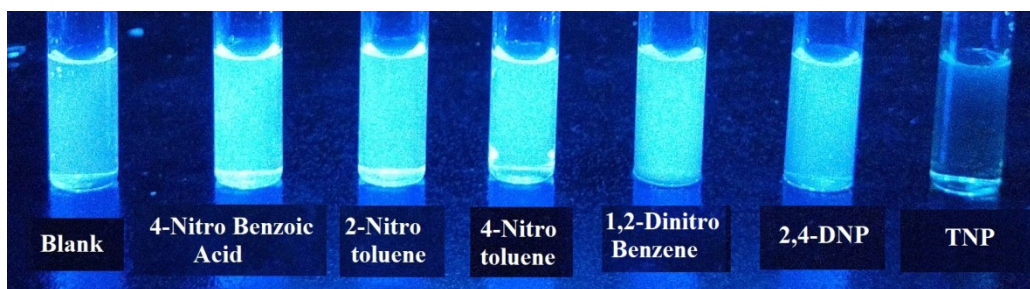


Fig. S10a Visual change of fluorescence intensity of Cd-MOF1 (in water) addition of nitro-explosives under UV light

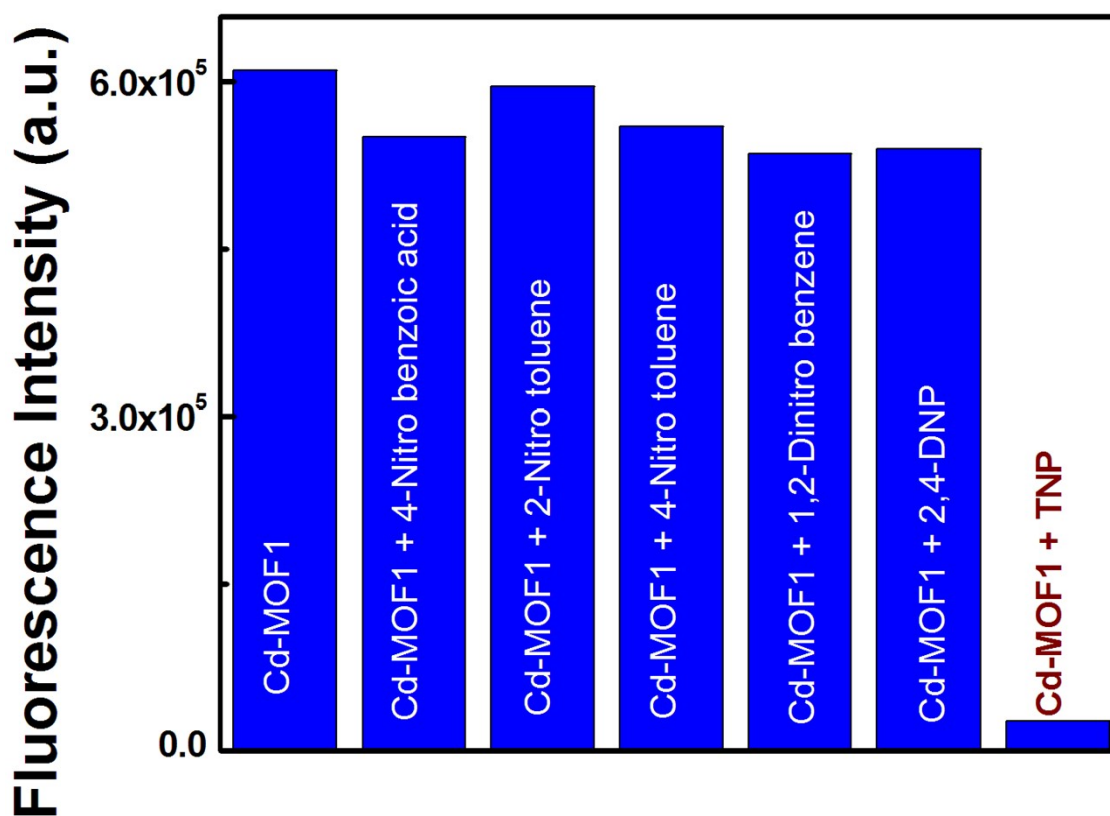


Fig. S10b Bar chart showing fluorescence response of Cd-MOF1 towards different nitroaromatics