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Highly Fluorescent 2D-BCNO Sheets based Chemical Sensor for Selective Detection of Explosive Dunnite and 4-Nitrophenol in Aqueous Medium

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1. XPS analysis

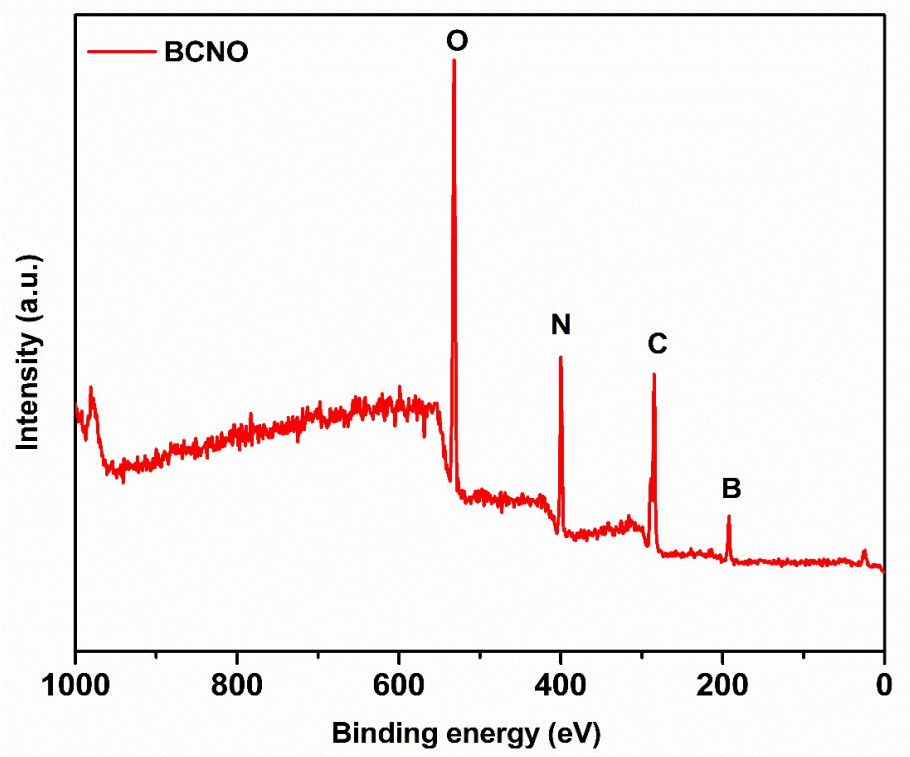

Fig. S1 XPS survey scan spectrum of 2D-BCNO sheets.

2. FT-IR

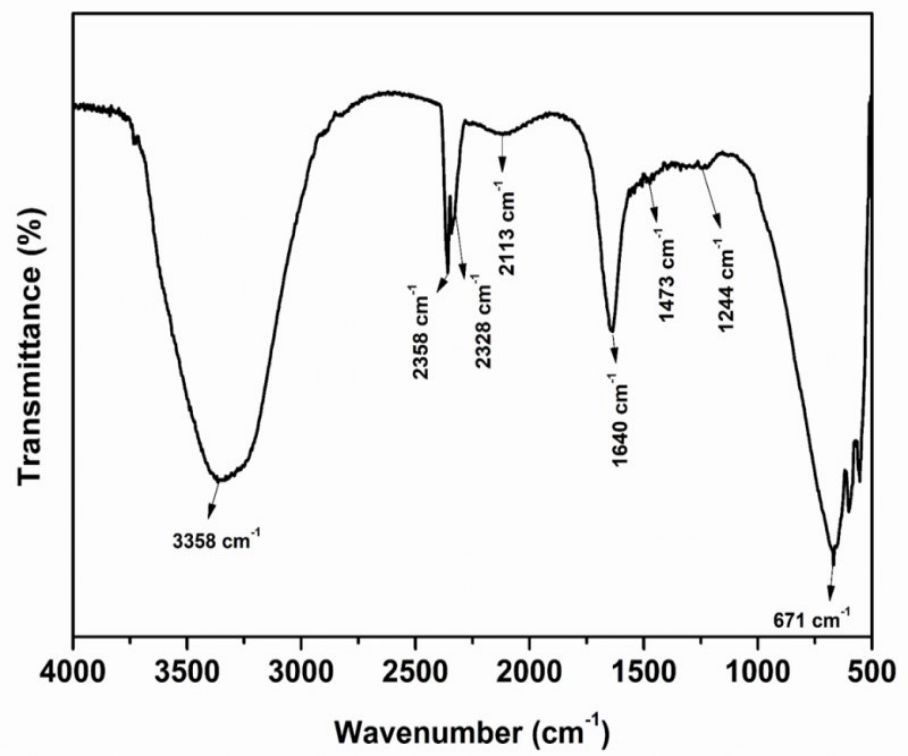

Fig. S2 FT-IR Spectrum of 2D-BCNO sheets.

3. Excitation dependent emission spectra

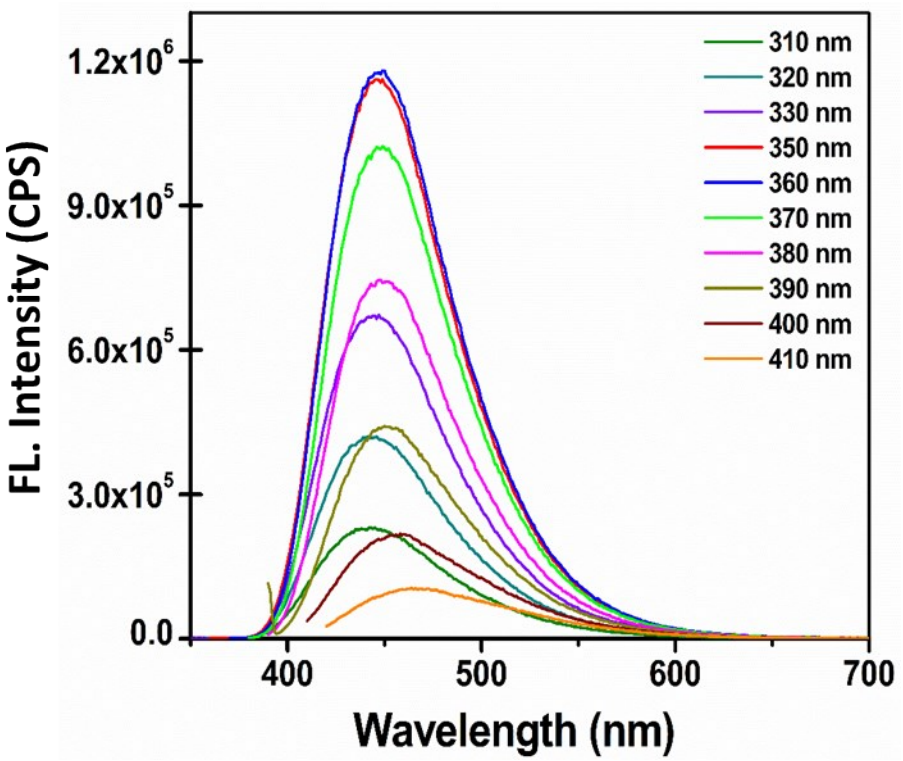

Fig. S3 Excitation dependent emission spectra of 2D-BCNO sheets in water medium.

4. pH dependent emission

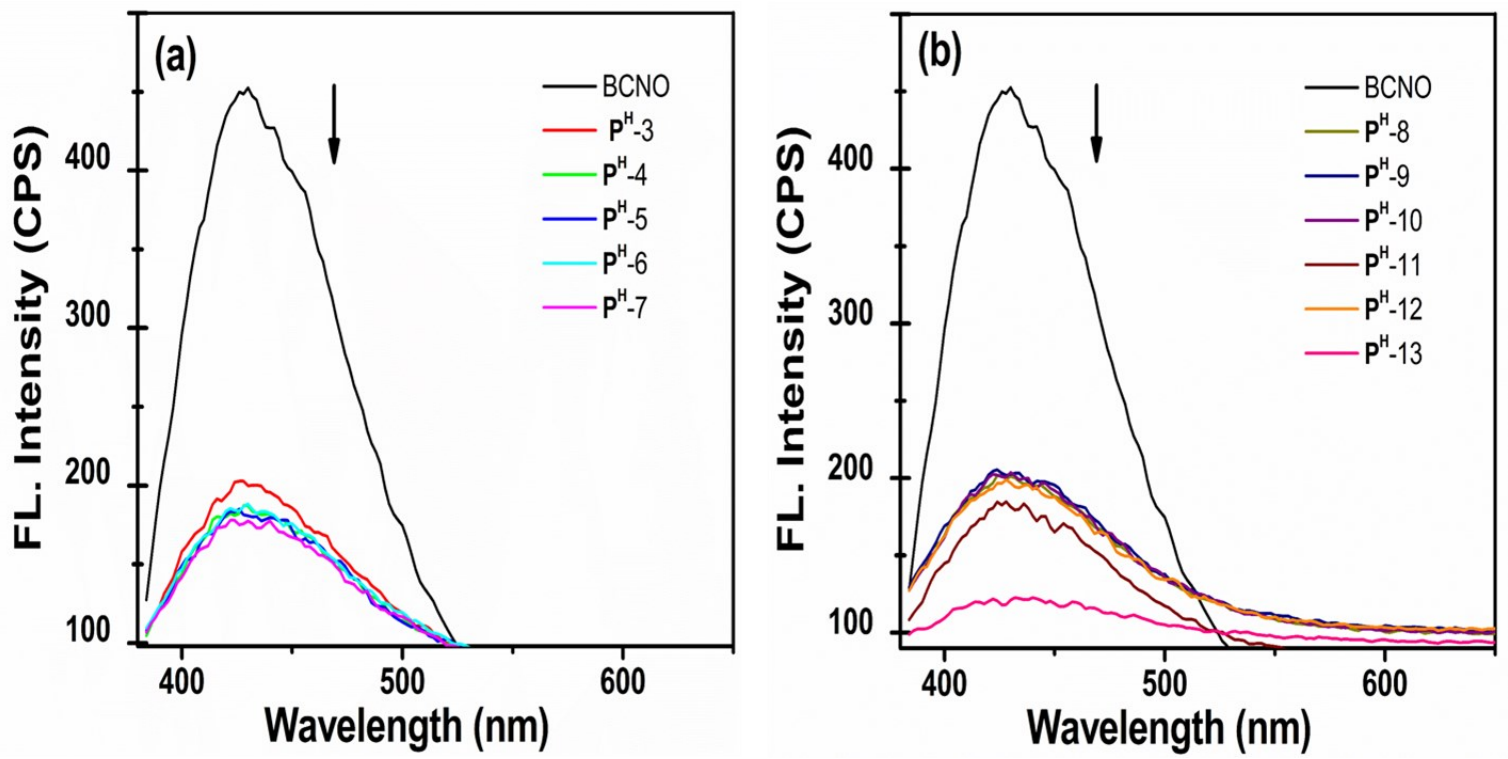

Fig. S4 pH dependent emission behaviour of 2D-BCNO sheets at wide range of pH **(a)** pH -1 to pH-7 and **(b)** pH -8 to pH-13.

5. Chemosensing studies

The 500µL of 2D-BCNO sheets was dispersed in 2mL of deionized water and taken into the cuvette. The emission of 2D-BCNO was recorded upon excitation at λ_{exc} = 360nm. To this solution, 10µL of different analayte concentrations were added and the resulting solution was mixed homogeneously and allows for 60 sec to have efficient interaction between 2D-BCNO sheets and analytes. The emission spectra were recorded after mixing thoroughly for each addition of analyte. The procedure was repeated for different nitro-aromatic compounds with different concentration to validate the selective and sensitive fluorescence quenching behaviour of 2D-BCNO sheets.

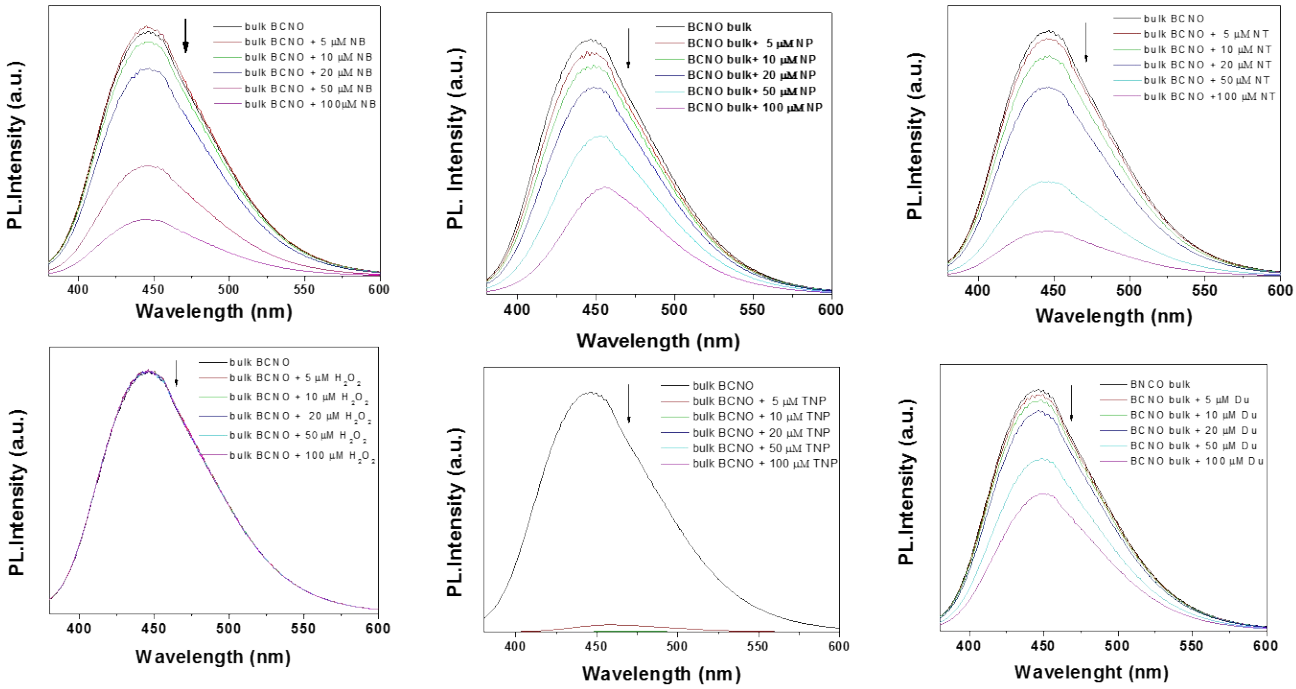

Fig. S5 Change in the fluorescence emission intensity of bulk BCNO upon addition of different concentrations of nitro analytes (0-100 µM).

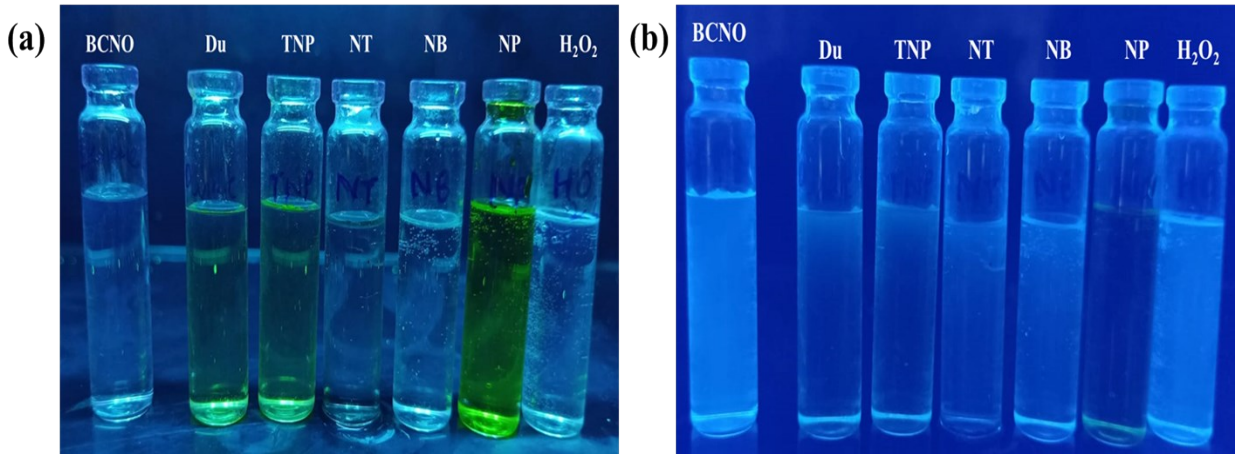

Fig. S6 Photographic images of 2D-BCNO sheets in aqueous medium with different nitro-analytes **(a)** under white light **(b)** under 365nm illumination.

6. LODs

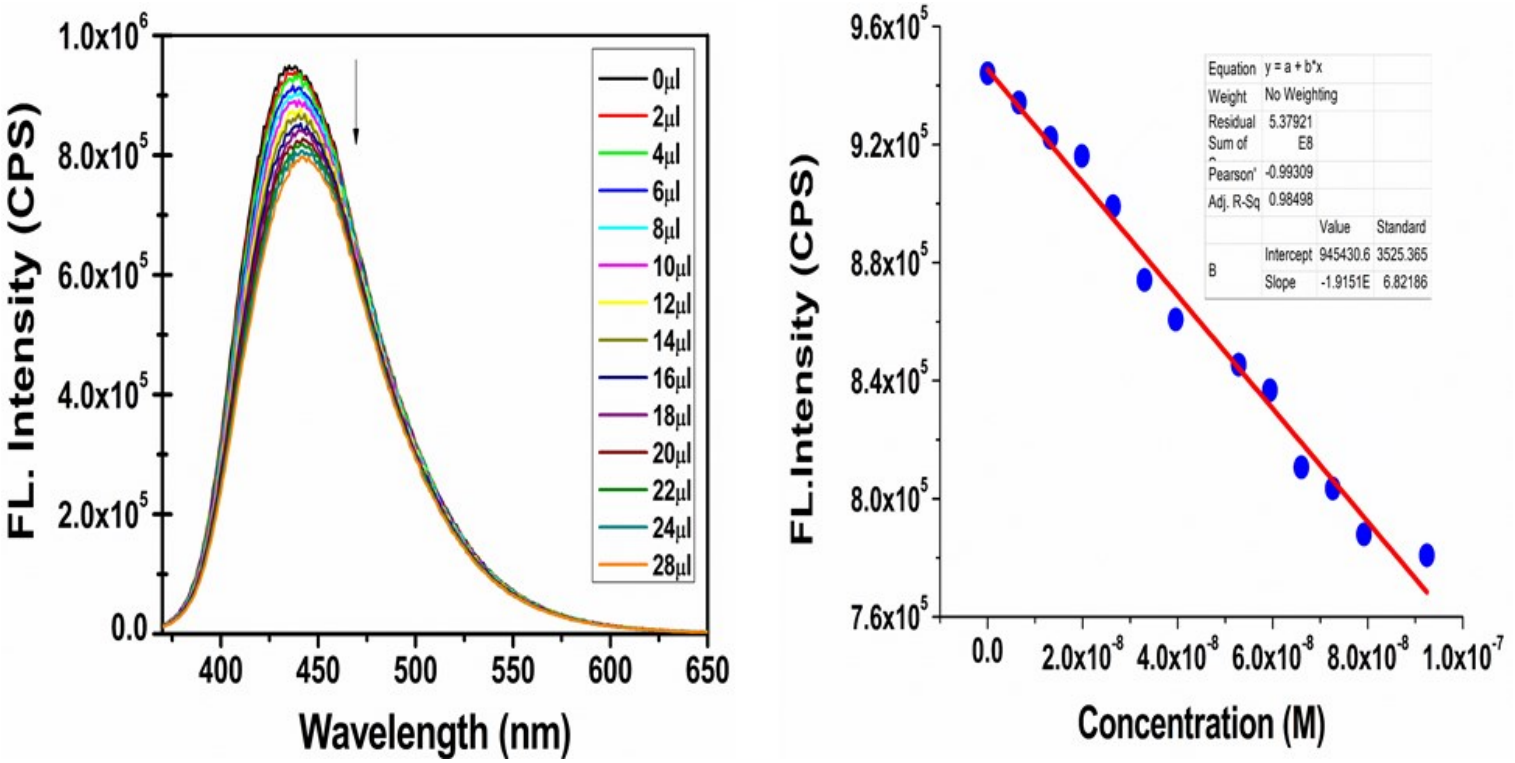

Fig. S7 Limit of detection (LOD) test for 4-Nitrophenol.

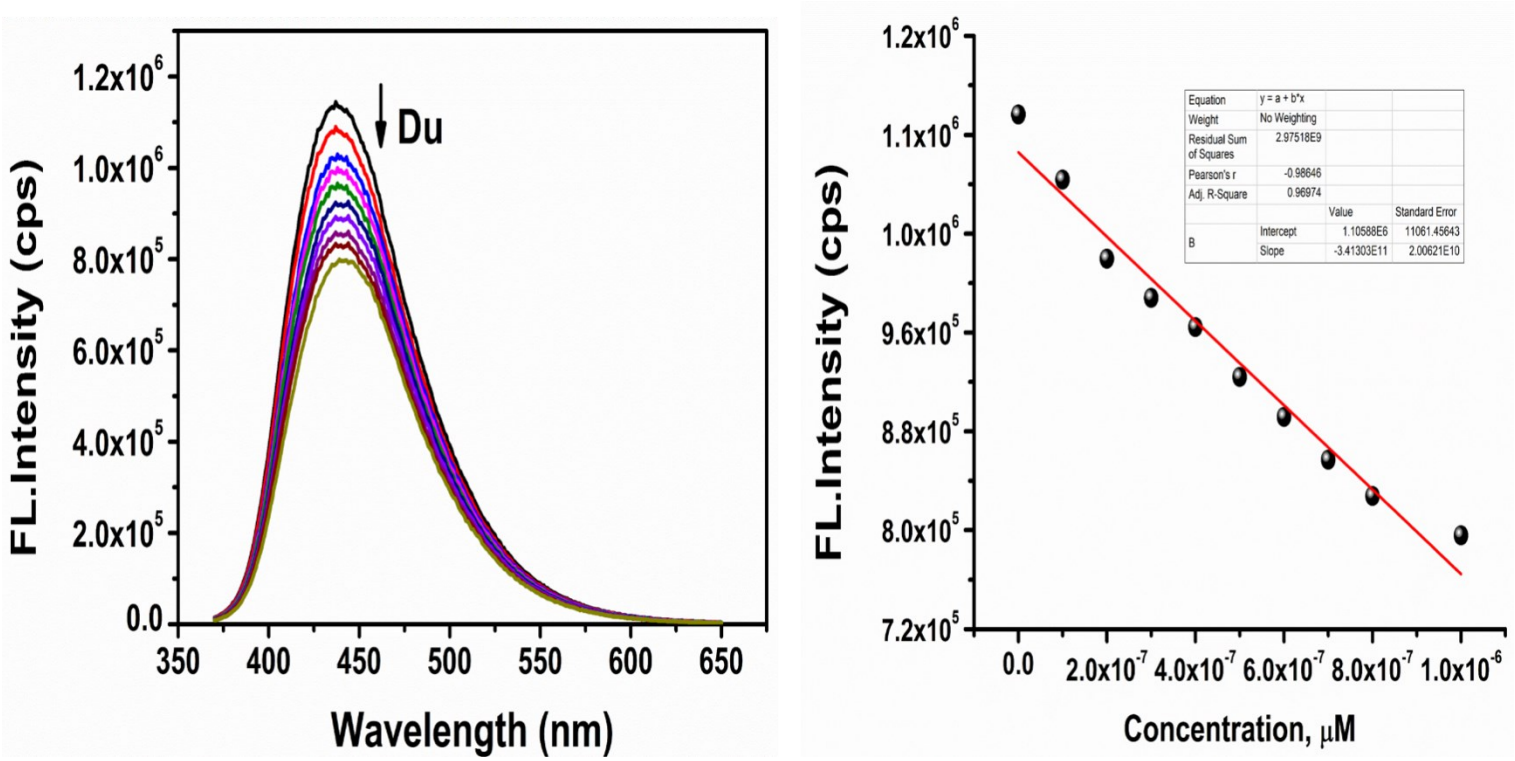

Fig. S8 Limit of detection (LOD) test for Dunnite.

7. Stability and Reusability test

The stability and reusability of 2D-BCNO sheets was tested by coating 2D-BCNO sheets on the glass substrate through spin coating method and dried at 60^{o}C. The emission spectrum of the coated substrates was recorded before and after addition of the analytes. Further, thin-film were washed with methanol and dried to remove the analyte particles (if any) adsorbed on the surface of the substrate. The emission spectrum of the glass substrate is collected again to understand its reusability. The process is repeated with similar procedure for different cycles and it was found that the emission of 2D-BCNO is retained after washing with methanol. After 6 cycles, we could see a small decrease in the emission intensity, which may arise due to release of few BCNO sheets

from the surface of the glass substrate. However, the rate of quenching efficiency remains same. Figure below shows the recycling ability of the coated film in different cycles.

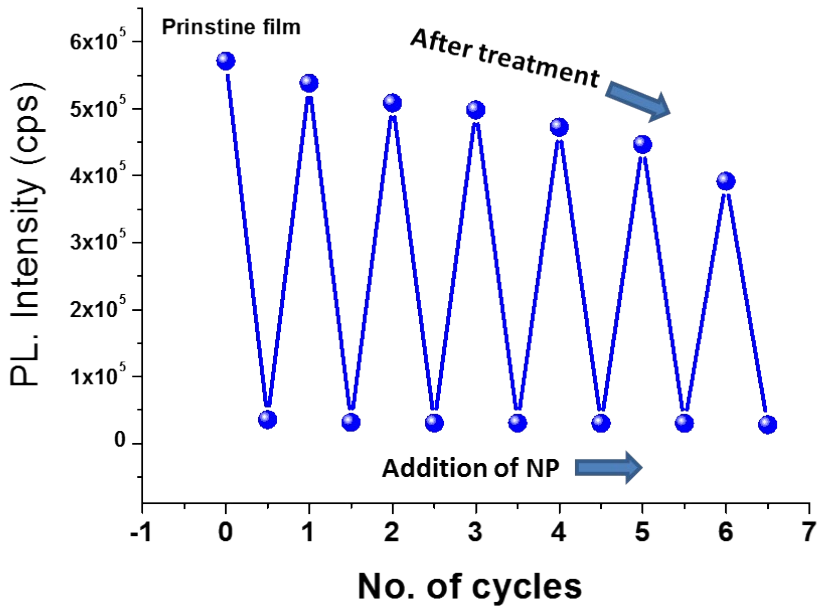

Fig. S9 The reversibility of 2D-BCNO coated thin films before and after addition of NP.

8. Fluorescence lifetime study

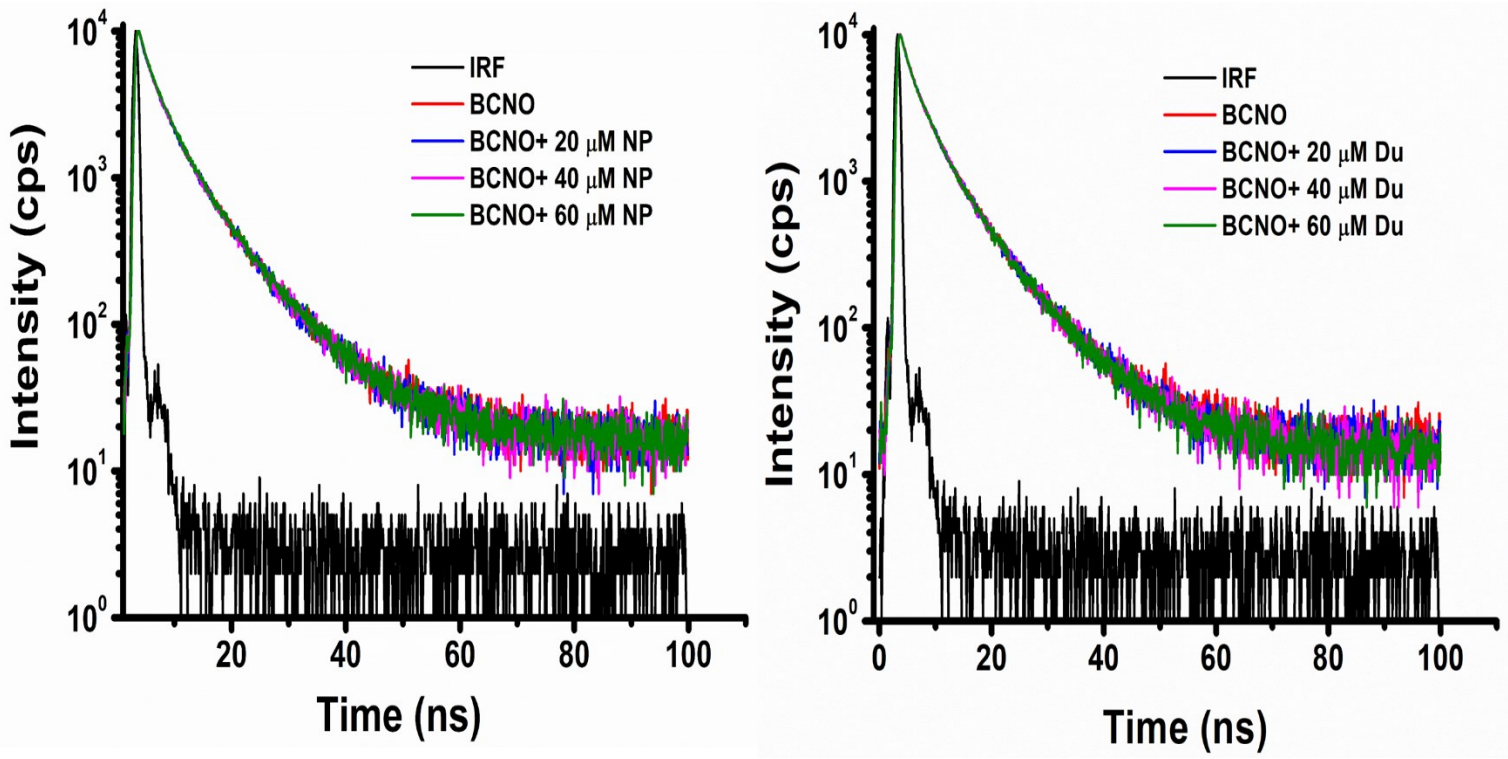

Fig. S10 Fluorescence decay lifetime of 2D-BCNO sheets treated with different concentrations of **(a)** NP and **(b)** Du.

9. Corrected fluorescence intensity

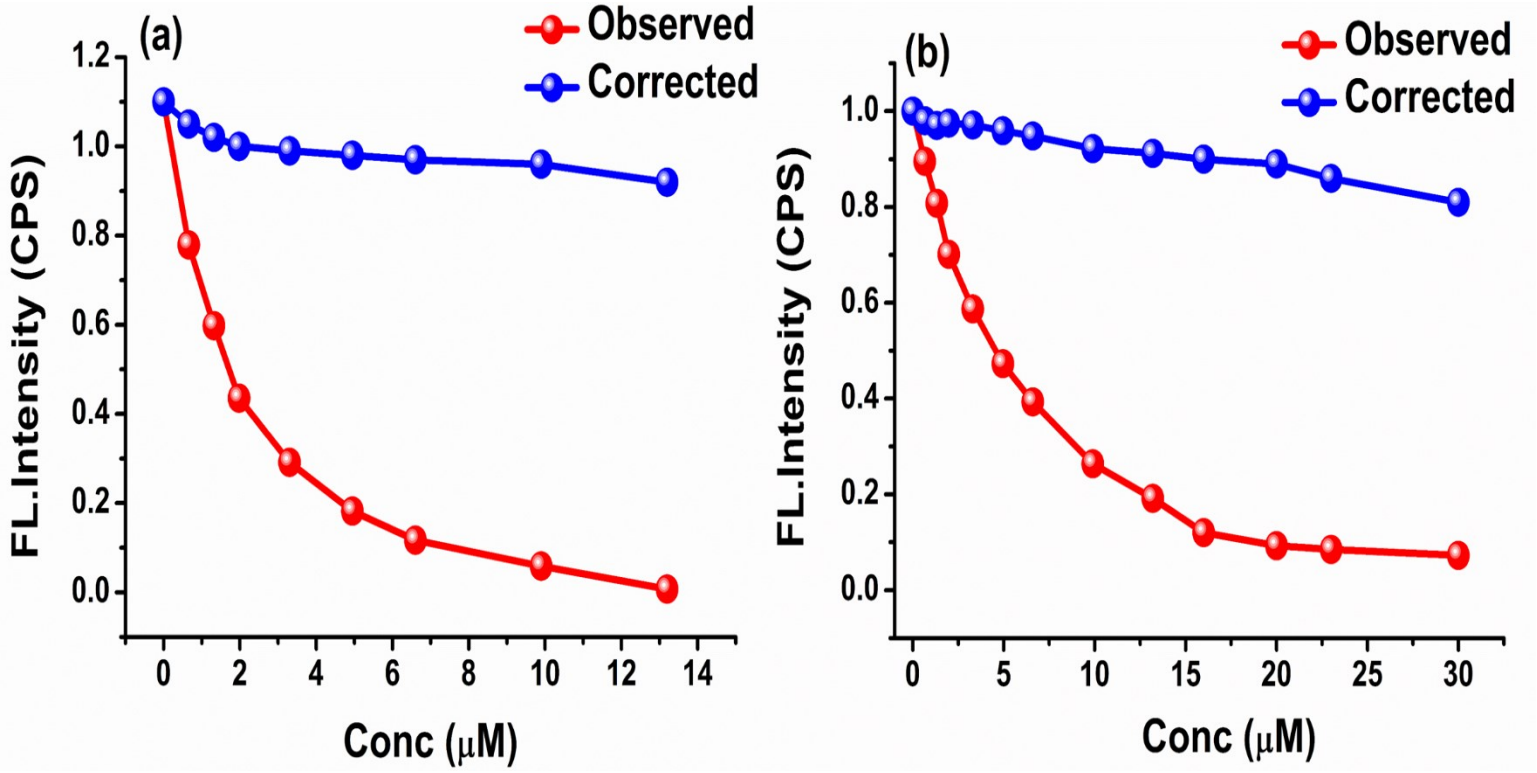

Fig. S11 The observed and corrected fluorescence intensity of 2D-BCNO sheets upon addition of different concentrations of **(a)** NP and **(b)** Du.

10. Absorption studies

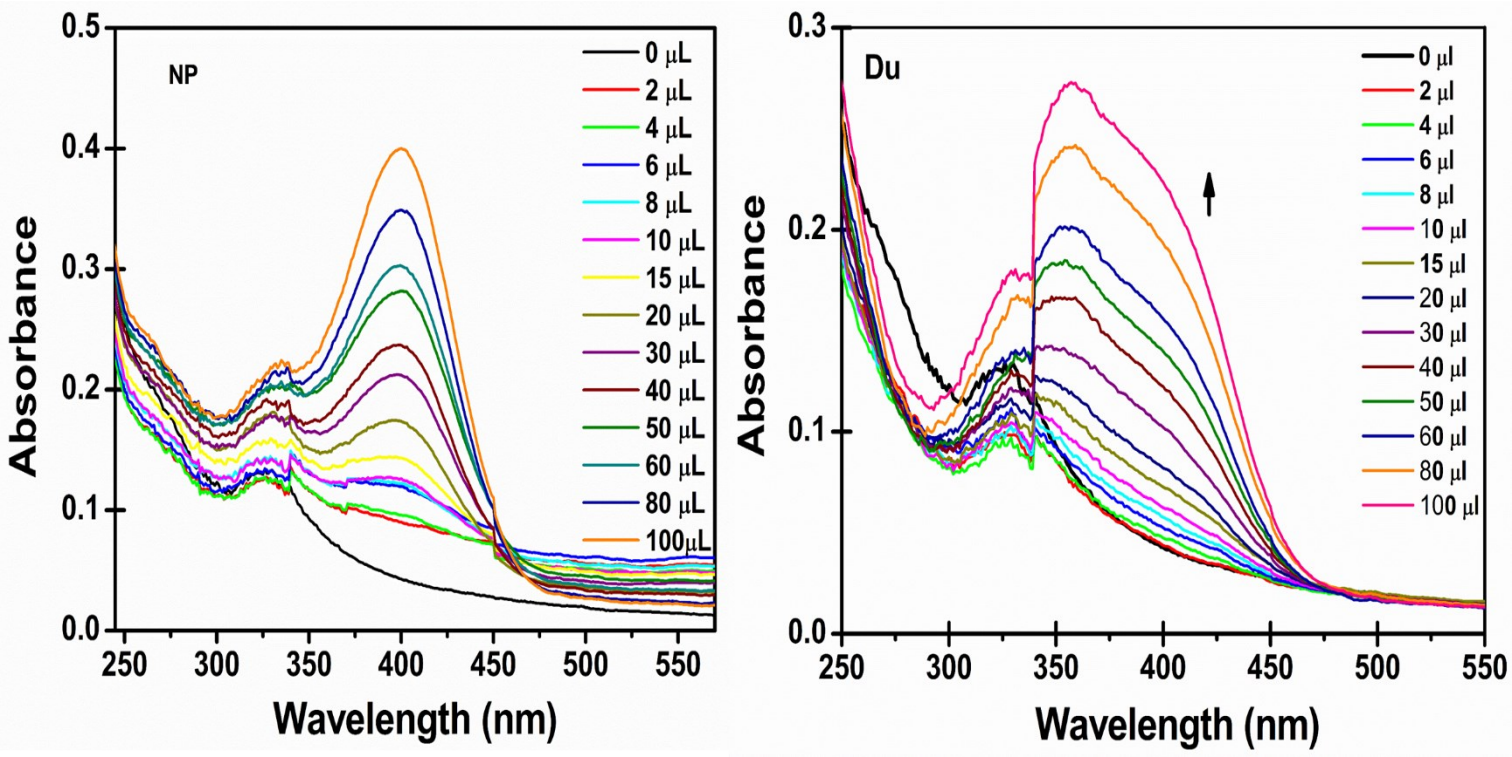

Fig. S12 Change in the absorption spectra of 2D-BCNO sheets upon addition of different concentrations of NP and Du in aqueous medium.

11. Morphological studies before and after addition of NP

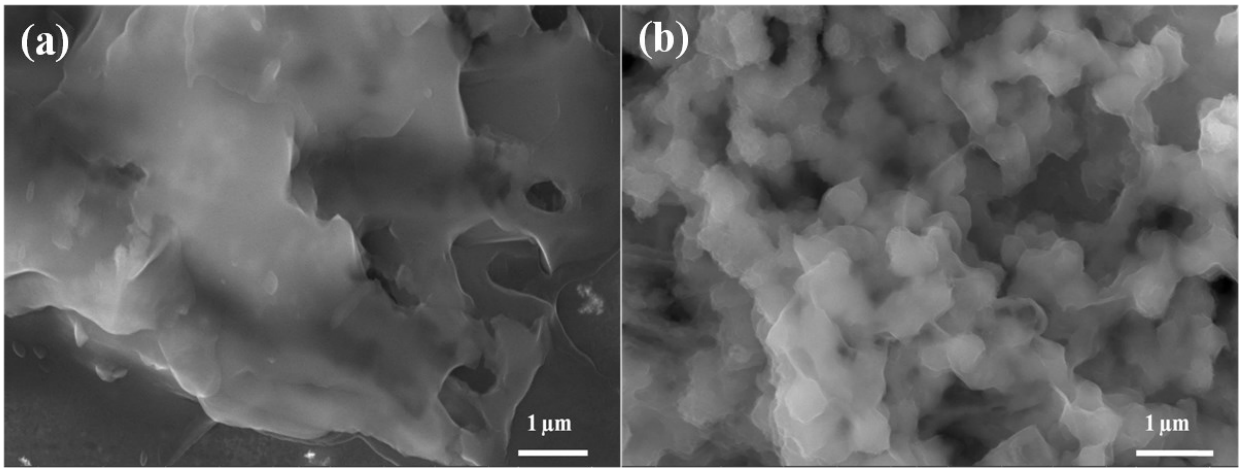

Fig. S13 FE-SEM image of 2D-BCNO sheets before and after addition of NP.

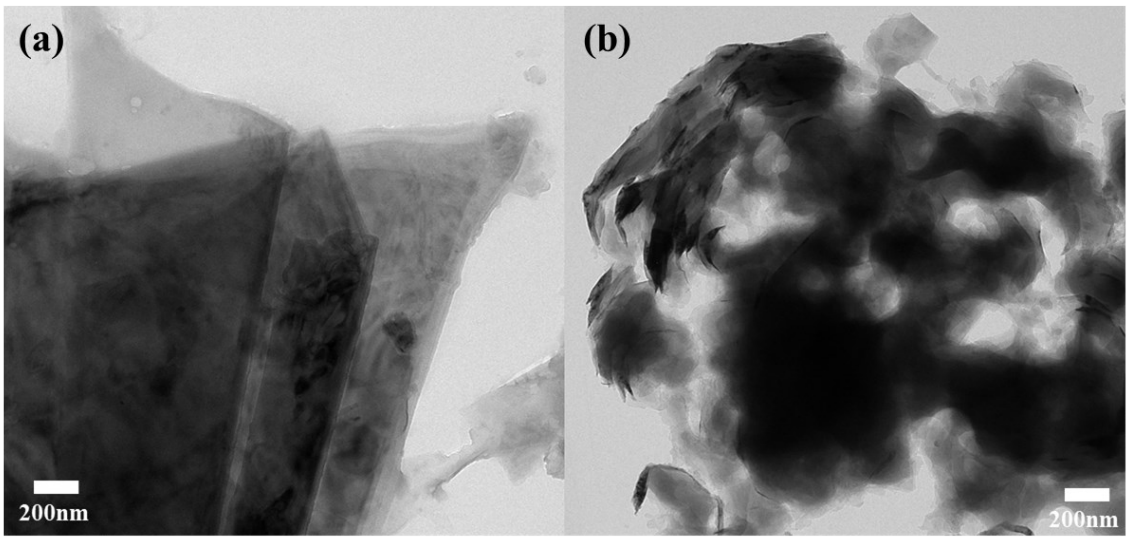

Fig. S14 HR-TEM image of 2D-BCNO sheets before and after addition of NP.

12. Time dependent emission

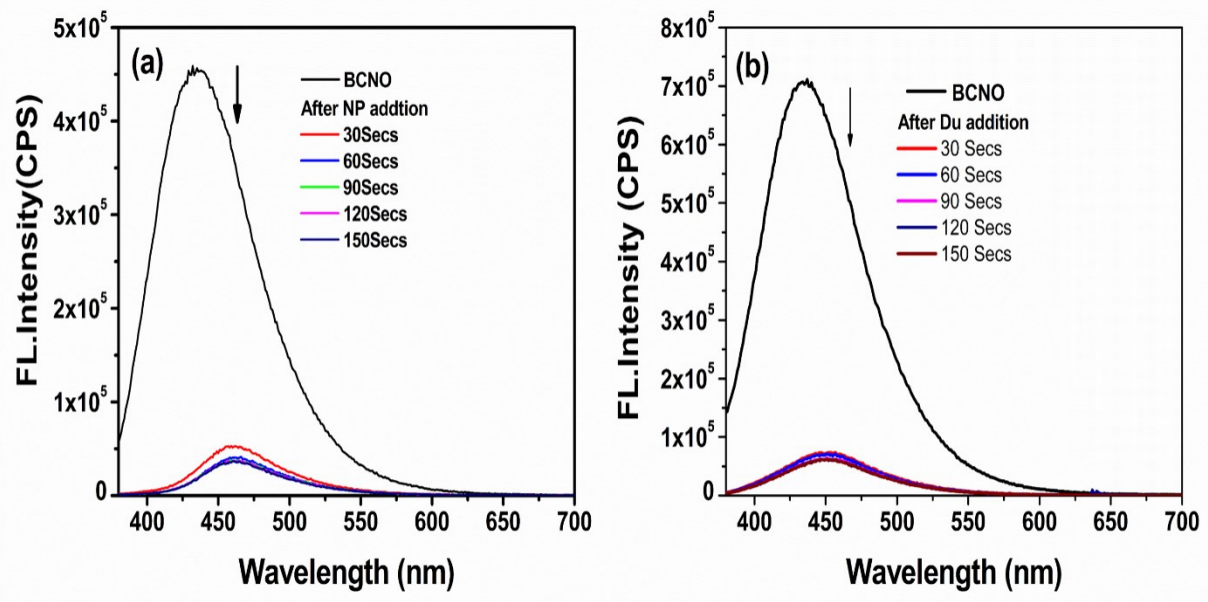

Fig. S15 Time dependent emission spectra of BCNO sheets upon addition of 16µM of **(a)** NP and **(b)** Du in aqueous medium

13. Effect of toxic anions, metal ions and interference with NP

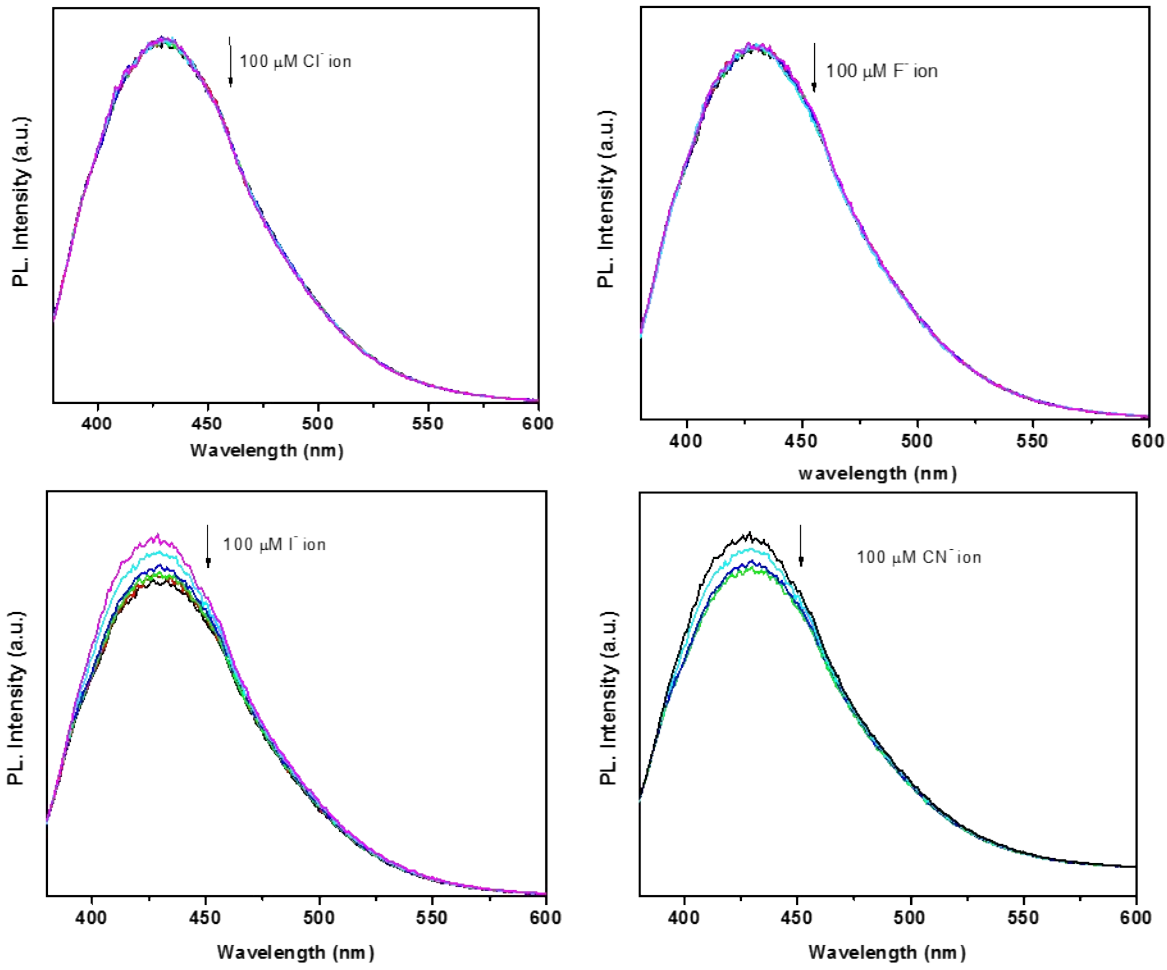

Fig. S16 Change in the fluorescence emission intensity of 2D-BCNO sheets upon addition of different anions (0-100 μM) in aqueous medium.

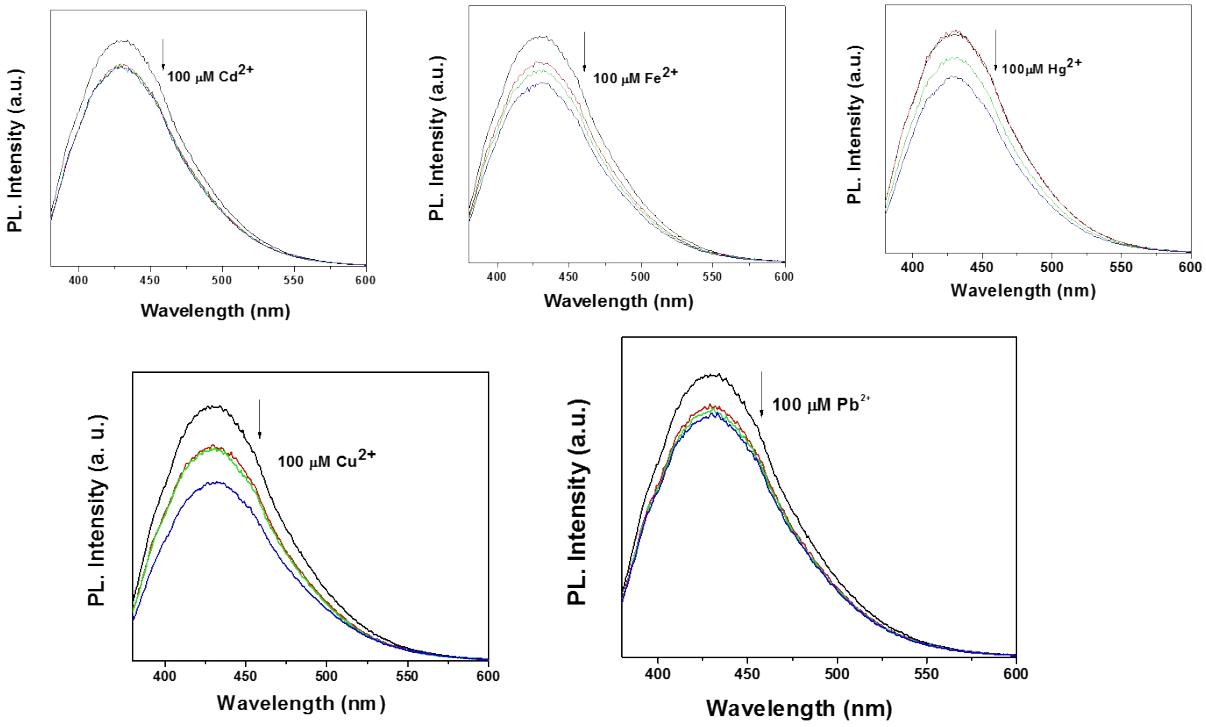

Fig. S17 Change in the fluorescence emission intensity of 2D-BCNO sheets upon addition of different metal ions (0-100 μM) in aqueous medium.

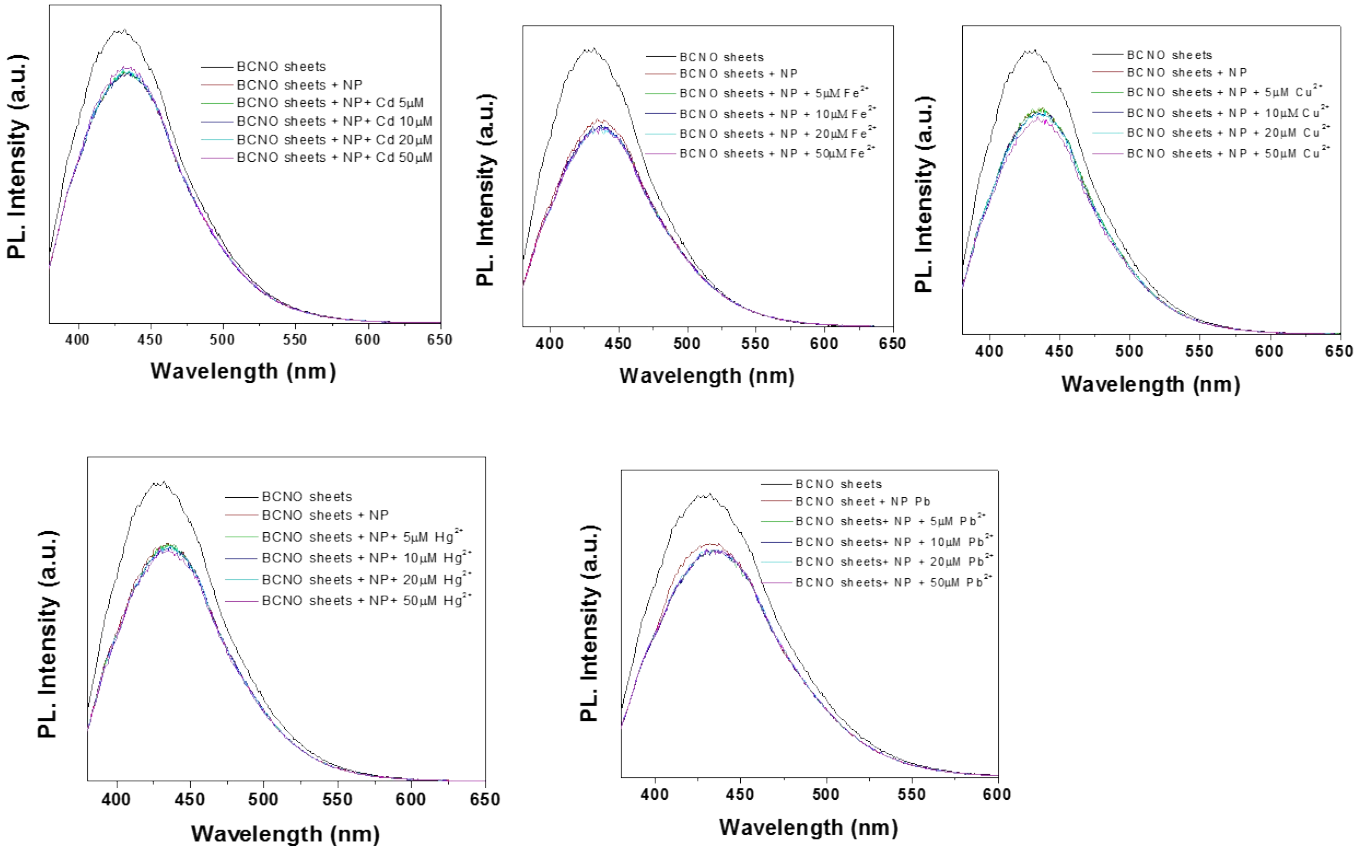

Fig. S18 Change in the fluorescence emission intensity of 2D-BCNO sheets upon addition of fixed concentration of 10μM of NP and addition of different concentrations of metal ions (0-50 μM) in aqueous medium.

Table. S1 Comparison of the various type of fluorophores reported in the literature for NP and Du detection.

S. No.	Type of fluorophore	Analyte	Limit of detection	Medium	Rate constant K_{sv} (M^{-1})	References
1	[Zn(opda)(bib)]n	2-NP	2.10×10^{-7}	aqueous solution	1.33×10^{7}	[1]
2	[Zn(ppda)(bib)(H2O)]n	2-NP	1.86×10^{-7}	aqueous solution	1.42×10^{7}	[1]
3	{[Zn2(μ3-OH)(cpta)(4,4′-bpy)]·H2O}n	4-NP	4.01×10^{-6}	aqueous solution	4.55×10^{4}	[2]
4	Au@S-GQD	4-NP	3.5×10^{-9}	aqueous solutions	--	[3]
5	fluorescent molecularly imprinted poly (ionic liquid) (FL-MIPIL)	4-NP	0.5 nM	DI water	--	[4]
6	BSA Au-NCs	4-NP	10 nM	DI water	--	[5]
7	Mn-doped ZnS quantum dots (QDs)	4-NP	76 nM	aqueous solutions	--	[6]
8	[Zr6O6(OH)2(CF3COO)2 (C11H5NO4)4(H2O)4]	4-NP	1.40 ppt	acetonitrile	--	[7]
9	QD@MIPs	4-NP	0.051 μM	DI water	--	[8]
10	C-dot	4-NP	0.028 μM	aqueous	--	[9]
11	MIP-coated carbon dot incorporated with YVO4: Eu3+*c* nanoparticles	4-NP	0.150 μM	water	--	[10]
12	MIP-coated GQDs	4-NP	0.064 μM	Na2CO3–NaHCO3	--	[11]

				buffer solution (pH 9)		
13	MIP-capped ZnO nanorods	4-NP	0.036 µM	Double distilled water	--	[12]
14	MIP-C-dots	4-NP	0.060 µM	deionized water	--	[13]
15	Zn-MOF-**1** ([Zn(L)(H2O)]・H2O)	4-NP	3.74 μM	DI water	--	[14]
16	Glycol modified Gd2O3	4-NP	3.9× 10^{-7} M to 7.1 × 10^{-7} M.	aqueous	--	[15]
17	GNCs@ BSA (Dual-emissive GNCs)	4-NP	0.0138 µM	DI water	--	[16]
18	S-GQDs	4-NP	0.7nM	DI water	--	[17]
19	CdTe@MIP	4-NP	40 nM	DI water	--	[13]
20	Zn-MOF	Dunnite	0.79 mM	water	9.77 × 10^{4} M^{-1}	[18]
21	2D-BCNO nano sheets	4-NP Dunnite	0.22ppb 2.1ppb	water	--	This work

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