Supplementary Information (SI) for Environmental Science: Nano.

Supporting information

Synthesis of Two-dimensional Bismuth Molybdenum Oxide (2D-BMO) nanosheets and their application as fluorescence probes for the detection of explosive nitroaromatic compound

Shams Ur Rehman[1], Sivakumar Musuvadhi Babulal[1], Muhammad Mustafa[1], Hui-Fen Wu*[1, 2, 3,4,5,6]

[1]Department of Chemistry, National Sun Yat-Sen University, Kaohsiung, 70, Lien-Hai Road, Kaohsiung, 80424, Taiwan

[2]School of Pharmacy, College of Pharmacy, Kaohsiung Medical University, Kaohsiung, 807, Taiwan

[3]Institute of Medical Science and Technology, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan

[4]School of Medicine, College of Medicine, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan

[5]Institute of Precision Medicine, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan

[6]Institute of BioPharmaceutical Sciences, National Sun Yat-Sen University, 80424, Taiwan

*Corresponding author, Phone: +886-7-5252000-3955; Fax: +886-7-5253909

Email: hwu@faculty.nsysu.edu.tw (Prof H.-F. Wu)

2.3. Instruments

The optical properties of the nanomaterials were assessed using an Evolution 201 UV-Vis spectrometer (Thermo SCIENTIFIC, USA). The morphology and structural characteristics were analyzed with a JEOL 3010 AEM High-resolution transmission electron microscope (HRTEM) and selected area electron diffraction (SAED) (JEOL, Japan). The crystallinity of the nanosheets was further investigated through X-ray diffraction (XRD, Bruker D8 Advance, Philips, Netherlands). X-ray photoelectron spectroscopy (XPS) was conducted to determine the chemical composition and oxygen vacancies, utilizing Auger electron spectroscopy with a field emission gun (JEOL, Japan). Atomic Force Microscopy (AFM) characterization was done by Seiko, Model: HV-300. The surface area and pore size of the nanosheets were measured using the Brunauer-Emmett-Teller (BET) method.

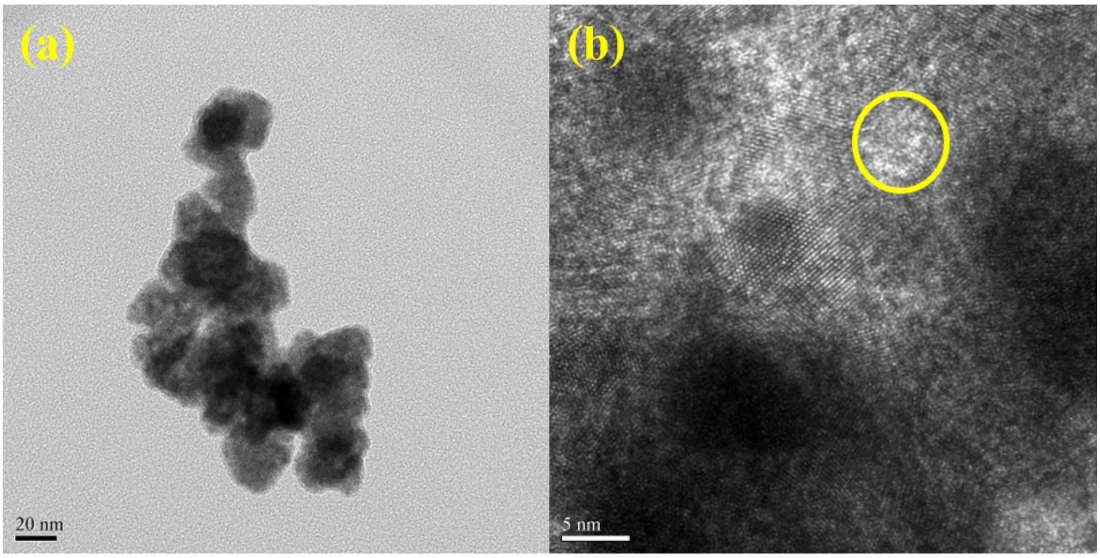


Fig. S1 (a) TEM and (b) HRTEM images of the 2D-BMO nanosheets

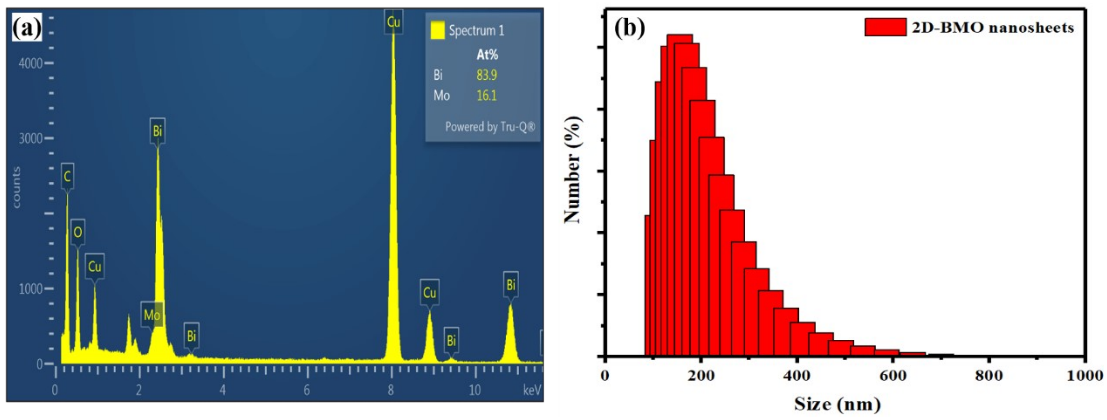


Fig. S2 (a) EDS spectra and (b) DLS to detect the size of the 2D-BMO nanosheets.

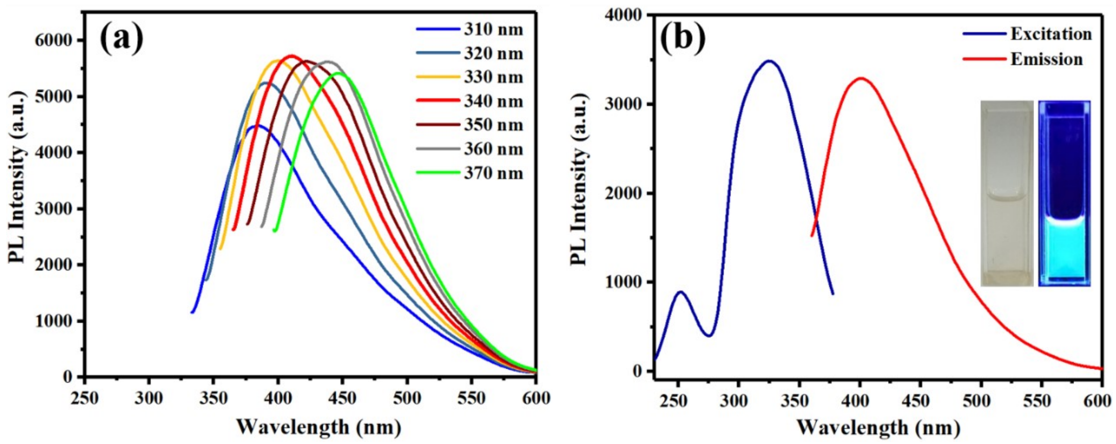


Fig. S3 (a) Emission spectra of the 2D-BMO nanosheets against excitation (310-370 nm), (b) excitation and emission spectra of the 2D-BMO nanosheets

S1. Quantum yield equation and calculation

The quantum yield of the synthesized material was calculated using the equation as below:

$$\varphi_{ZnO_{2D-BMO}} = \varphi_{Q.S} \times \frac{F(AUC)_{2D-BMO}}{F(AUC)_{Q.S}} \times \frac{Absorbance_{Q.S}}{Absorbance_{2D-BMO}} \times \frac{\eta_{2D-BMO}}{\eta_{Q.S}}$$

where φ is Quantum yield, Q.S. = Quinine sulfate (reference), F (AUC) = Fluorescence Area under the curve, Absorbance = Absorbance at 370 nm, η = Solvent refractive index of the sample (water: 1.333).

The quantum yield of 2D-BMO was calculated using the values as:

$\varphi_{Q.S}$ = 54.6%, F(AUC)$_{2D\text{-}BMO}$ = 10866.9, F(AUC)$_{Q.S}$ = 60,260.0, Absorbance$_{Q.S}$ = 2.9, Absorbance$_{2D\text{-}BMO}$ = 0.7, $\eta_{2D\text{-}BMO}$ = 1.4, and $\eta_{Q.S}$ = 1.3 (water as a solvent)

S2. Quenching efficiency equation

The quenching efficiency (QE) of ferritin and all other interfering biomolecules was calculated using the equation below:

$$QE = \frac{(I_0 - I)}{I_0} \times 100$$

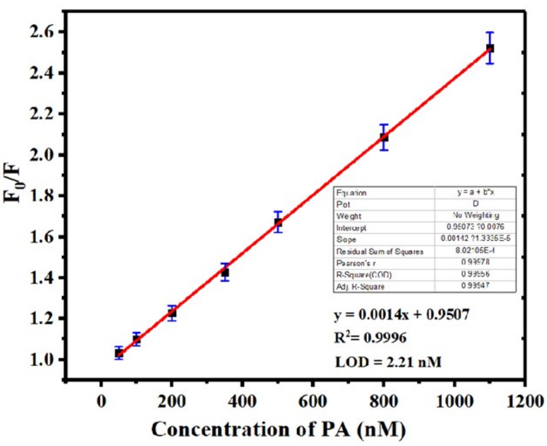
Where I_0 and I are the fluorescence intensities of 2D-BMO nanosheets without and with analyte, respectively.

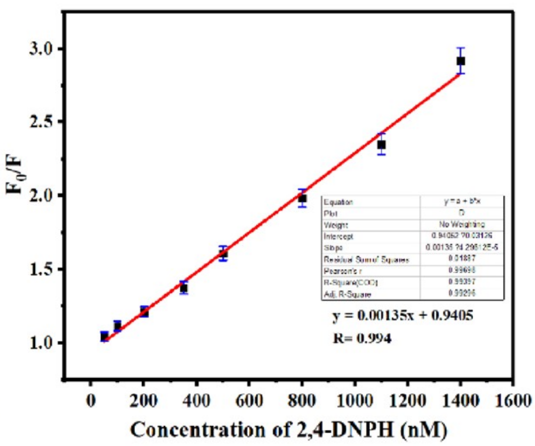
S3. LOD calculations

The LOD values for PA and 2,4-DNPH were calculated by the following formulas.

LOD = 3.3*SD/S

SD = Intercept/1000[1]





Calculation for PA:

Slope =0.00142

Intercept = 0.951

SD = 0.950/1000 = 0.00095

LOD = 3.3*0.000951/0.00142 = 2.21 nM

Calculation for 2,4-DNPH:

Slope =0.00135

Intercept = 0.9405

SD = 0.9405/1000 = 0.0009405

LOD = 3.3*0.000941/0.00135 = 2.30 nM

S.4 Quenching constant (Ksv) calculation

Stern-Volmer equation:

$F_0/F = 1 + Ksv\ [Q]$

F_0 and F indicate the fluorescence intensities before and after introducing the quencher, respectively, Ksv is the quenching constant, and [Q] indicates the quencher concentration[2,3].

Quenching constant for PA (Ksv_{PA})

The calculated Stern-Volmer equation for the PA given above is:

y= 0.0014x + 0.950

so the calculated **Ksv_{PA}** value is **0.0014**

Quenching constant for PA (Ksv_{PA})

The calculated Stern-Volmer equation for the PA given above is:

y= 0.00135x + 0.950

so the calculated **$Ksv_{2,4\text{-}DNPH}$** value is **0.00135**

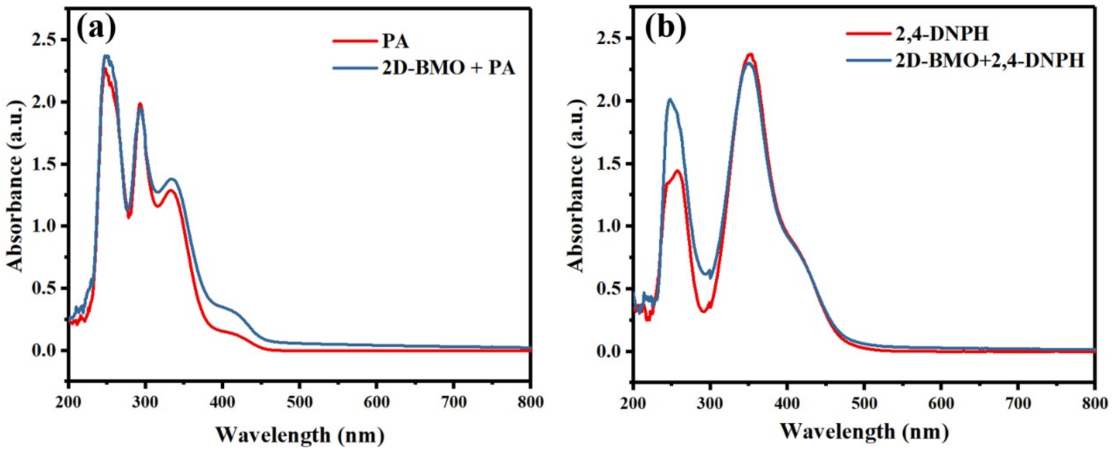


Fig. S4 (a) PA, and PA with the 2D-BMO nanosheets, (b) 2,4-DNPH, and 2,4-DNPH with the 2D-BMO nanosheets UV-visible absorption spectra

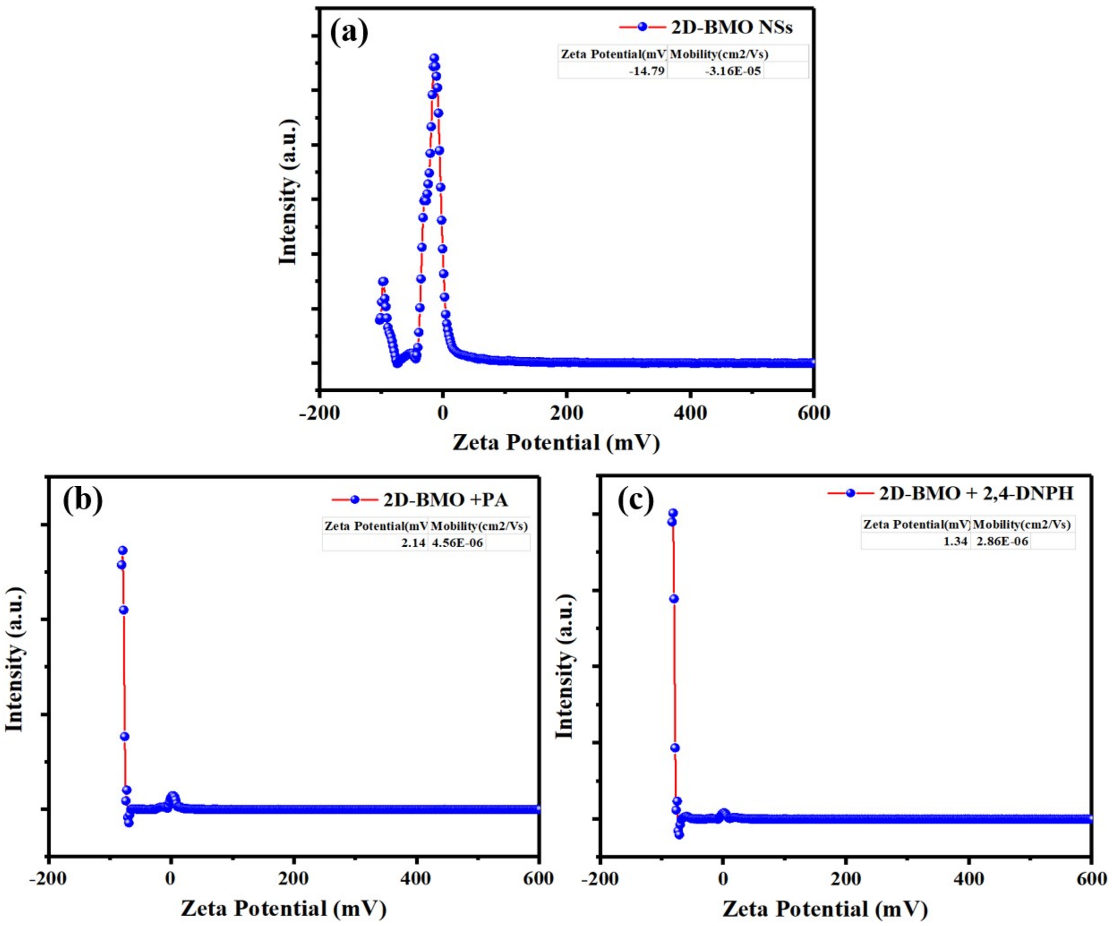


Fig. S5 (a-c) Zeta potential of 2D-BMO nanosheets, 2D-BMO nanosheets with the PA, and 2D-BMO nanosheets with the 2,4-DNPH respectively.

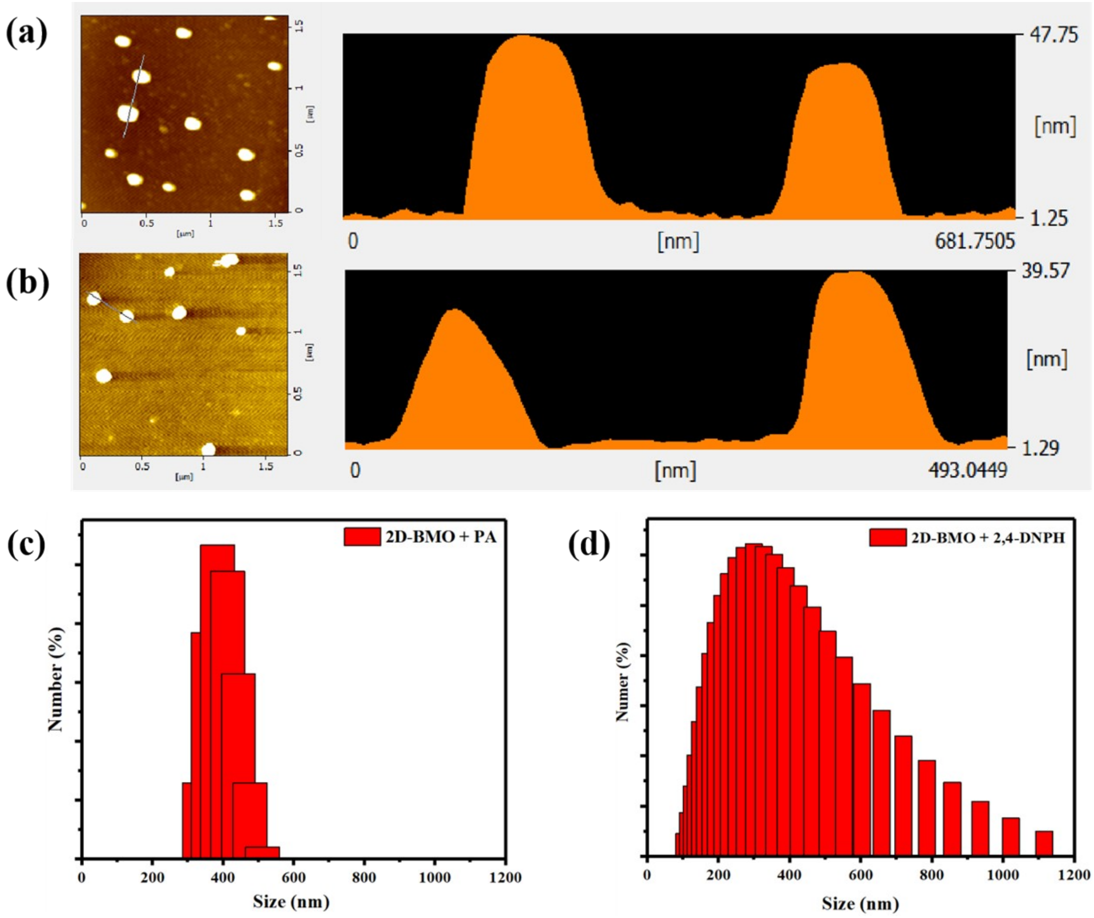


Fig. S6 (a,b) AFM topography and height profile, (c,d) DLS size of 2D-BMO with the PA and 2D-BMO with the 2,4-DNPH respectively.

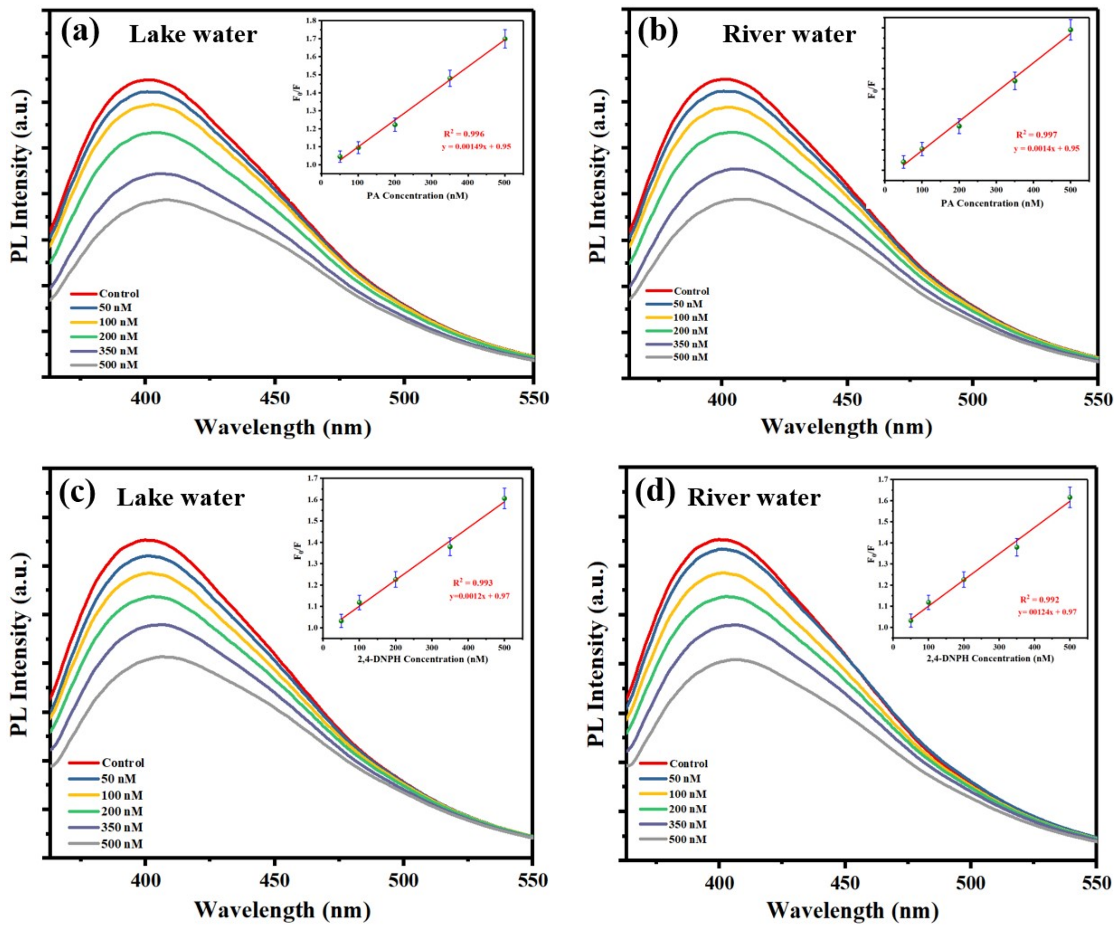


Fig. S7 Real sample studies of PA in (a) lake water, and (b) river water. Real sample studies of 2,4-DNPH in (c) lake water, and (d) river water.

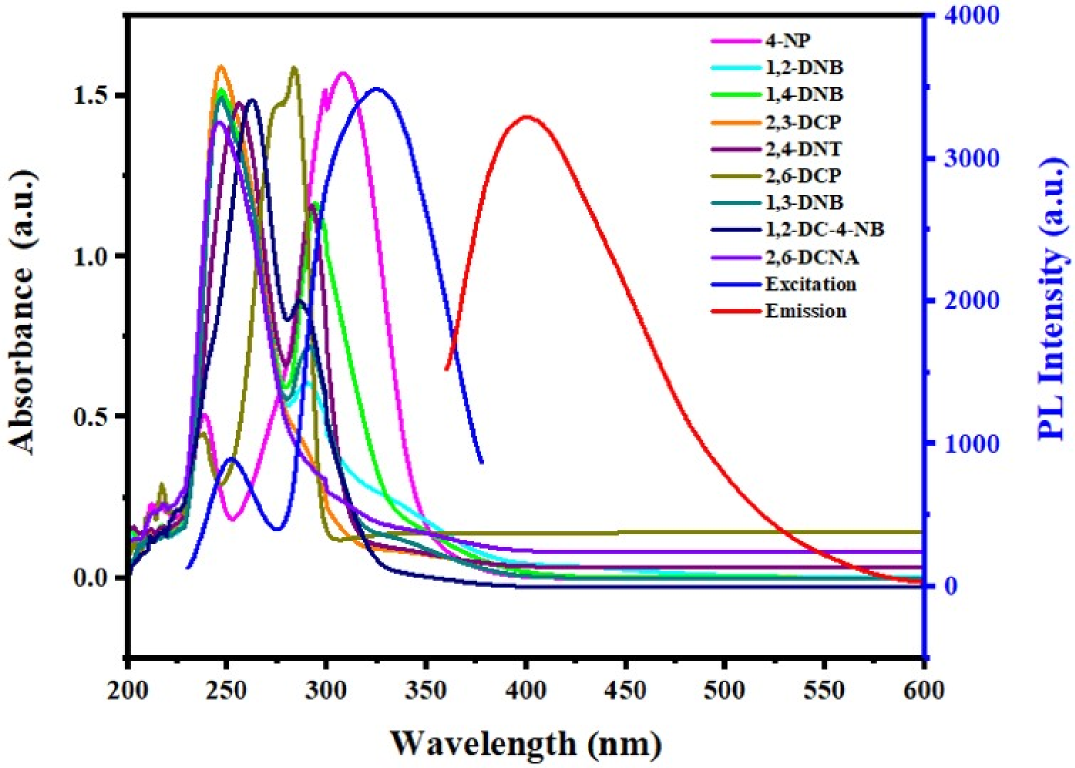


Fig. S8 Absorption spectra of nitroaromatic and excitation and emission spectra of the 2D-BMO nanosheets

Table S1. Comparison of different chemosensors with 2D-BMO nanosheets from literature for the detection of PA and 2,4-DNPH

Material	**Method**	**Nitroaromatic compound**	**LOD**	**References**
Zn-MOF	Fluorescence	2,4-DNPH PA	100 nM 500nM	[2]
BODIPY derivatives	Fluorescence	2,4-DNPH	1.06 μM	[4]
p-PABA-MnO_2	Electrochemical	2,4-DNPH	0.08 μM	[5]
CdTe QDs	Fluorescence	2,4-DNPH	0.23 ng/mL	[6]
Thiobarbituric acid based	HPLC-UV	2,4-DNPH	0.25 ng/ml	
2D ONs	Fluorescence	2,4-DNPH	0.1 μM	[3]
Carbon nanoparticles	Fluorescence	PA	0.25 μM	[7]
NCDs Malic acid and Urea	Fluorescence	PA	33 nM	[8]
palladium-based macro-cycles	Fluorescence	PA	0.2 μM	[9]
PFAM	Fluorescence	PA	57.8 nM	[10]
Phen-SnO_2 Nanosheets	Fluorescence	PA	0.011 μM (11 nm)	[11]
2D-BMO nanosheets	Fluorescence	2,4-DNPH PA	2.30 nM 2.21 nM	**This work**

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