

***Supporting information for***

**Green synthesis of an ionic porous organic polymer for efficient capture of environmentally toxic  $\text{MnO}_4^-$  and  $\text{I}_3^-$  from water**

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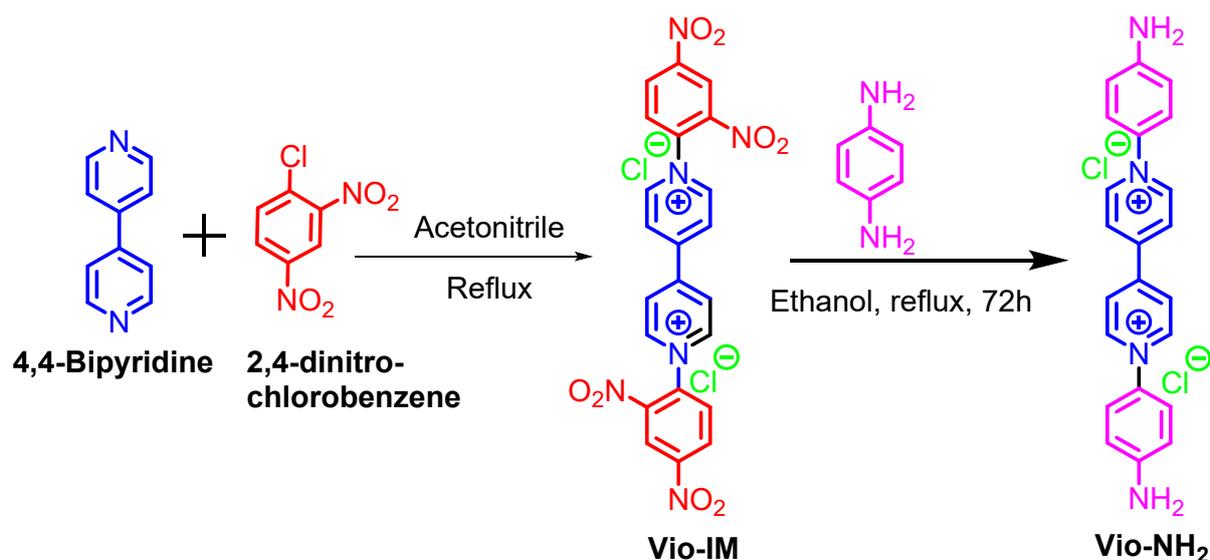
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### Procedure for the Synthesis of Monomer (Vio-NH<sub>2</sub>)



Scheme-S1: Synthesis of the Vio-IM and Vio-NH<sub>2</sub>

The monomer (**Vio-NH<sub>2</sub>**) was synthesized in two steps. First, Vio-IM was obtained by reacting 4,4'-bipyridine (4 g, 25.60 mmol) and 1-chloro-2,4-dinitrobenzene (26 g, 89.60 mmol) in 150 mL of anhydrous acetonitrile under refluxing conditions and inert atmosphere for 72 hours (Scheme-S1). Subsequently, the mixture was filtered and the residue obtained was thoroughly washed with acetonitrile and diethyl ether. The solid thus obtained was air-dried to yield pure Vio-IM (75%). Next to synthesize Vio-NH<sub>2</sub>, Vio-IM (500 mg, 0.89 mmol) and 1,4-diaminobenzene (289 mg, 2.67 mmol) were dissolved in 250 mL absolute ethanol and the resulting solution was refluxed for 72 h. The progress of the reaction was monitored by thin-layer chromatography (TLC). The solution was then concentrated to 50 mL using a rotary evaporator. Later, the reaction mixture was poured into 500 mL of tetrahydrofuran (THF). After 2.5 hours, a dark brown solid was formed which was collected by filtration (under reduced pressure) and washed with THF (10 mL × 5). The resulting solid was dried in a vacuum oven at 45 °C for 5 hours to yield Vio-NH<sub>2</sub> (68 %). The successful synthesis of Vio-NH<sub>2</sub> was indicated from its <sup>1</sup>H-NMR (Fig. S1).

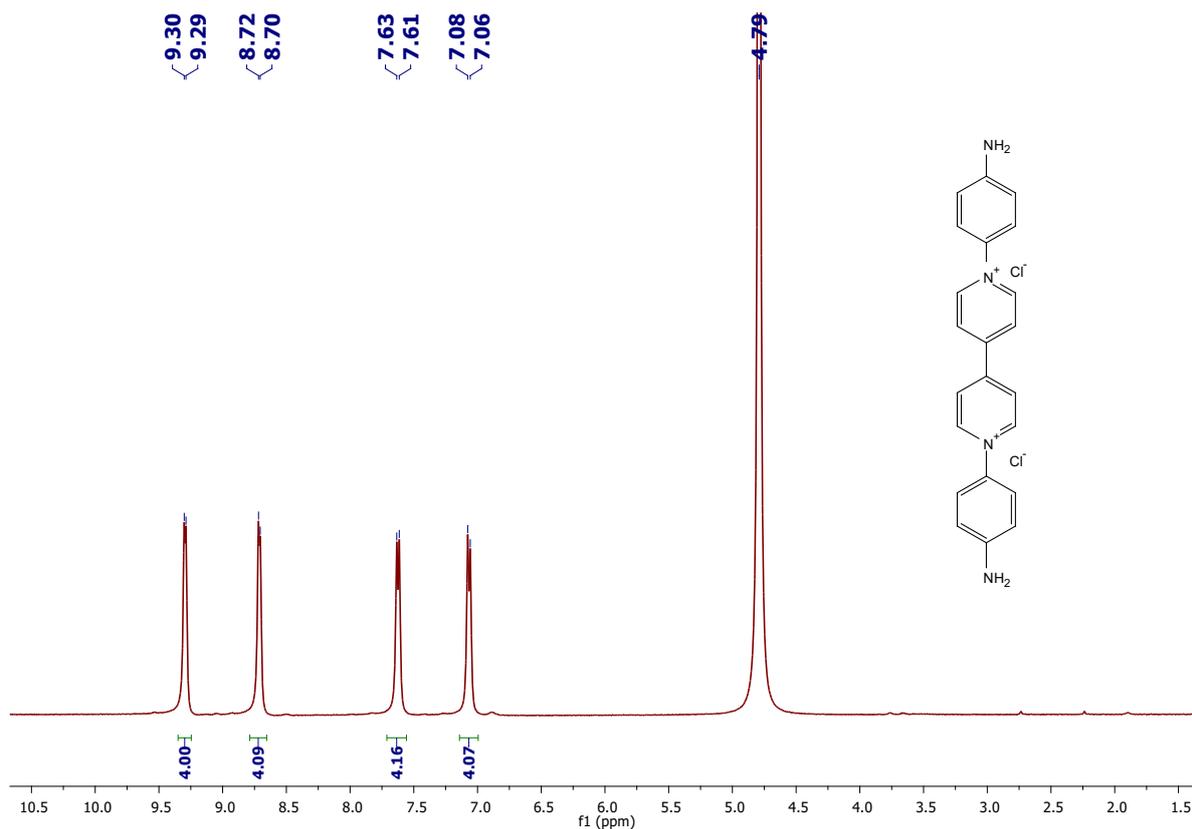


Figure -S1:  $^1\text{H}$ - NMR spectrum of Vio-NH<sub>2</sub>

### Procedure for the Synthesis of iPOP-6

In a 250 mL round-bottom flask, 1.5 mmol of Vio-NH<sub>2</sub> is suspended in 100 mL of water along with 0.2 mL of concentrated HCl, and the mixture is stirred for 15 minutes at a temperature of 0–5 °C. To this cooled solution, 30 mL of an aqueous solution of sodium nitrite (3.1 mmol) is added, and the reaction mixture is stirred for an additional 25 minutes to ensure the complete conversion of Vio-NH<sub>2</sub> to its corresponding diazonium salt. Following this, the mixture is neutralized using a dilute solution of Na<sub>2</sub>CO<sub>3</sub>. Subsequently, 30 mL of an aqueous solution containing phloroglucinol(PG) (1 mmol) and Na<sub>2</sub>CO<sub>3</sub> (3 mmol) is added to the reaction mixture, which is maintained at 0–5 °C. The resultant mixture is stirred for 24 hours, leading to the precipitation of the desired product. The precipitate is collected using a glass frit, then washed sequentially with water, DMF, acetone, methanol, THF and Dil HCl. Further purification is achieved using a Soxhlet extractor with methanol and THF as solvents. Finally, the obtained material is dried in a vacuum oven at 120 °C for 20 hours, yielding iPOP-6 (76%) as a dark powder.

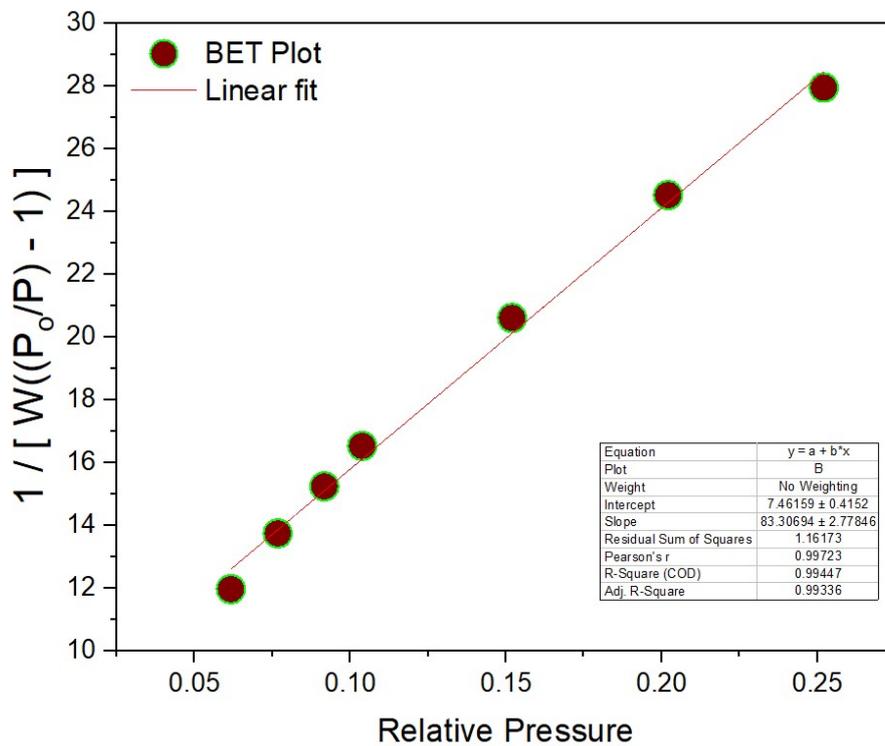


Figure S2 : BET plot of iPOP-6

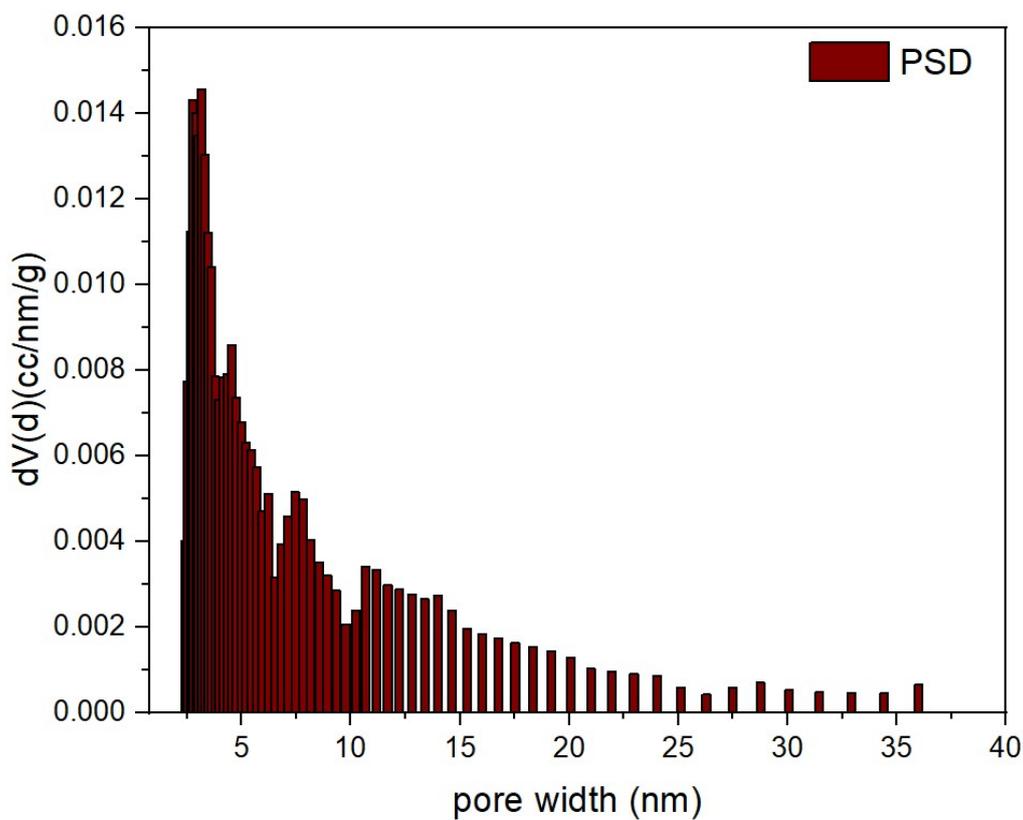


Figure S3: NLDFT pore size distribution plot of iPOP-6

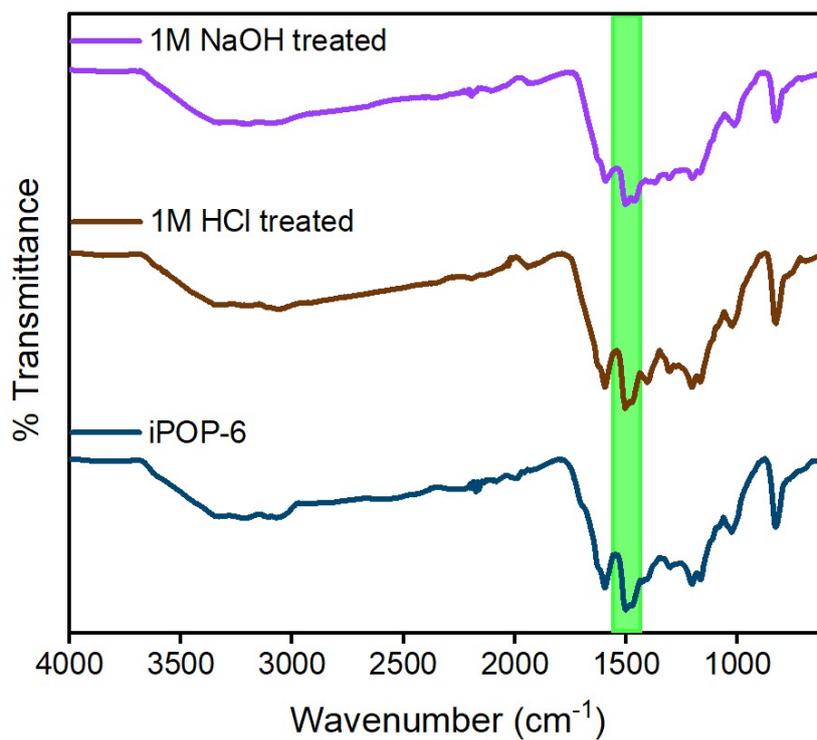


Figure S4: FTIR spectrum of the acid base treated iPOP-6 with pristine iPOP-6

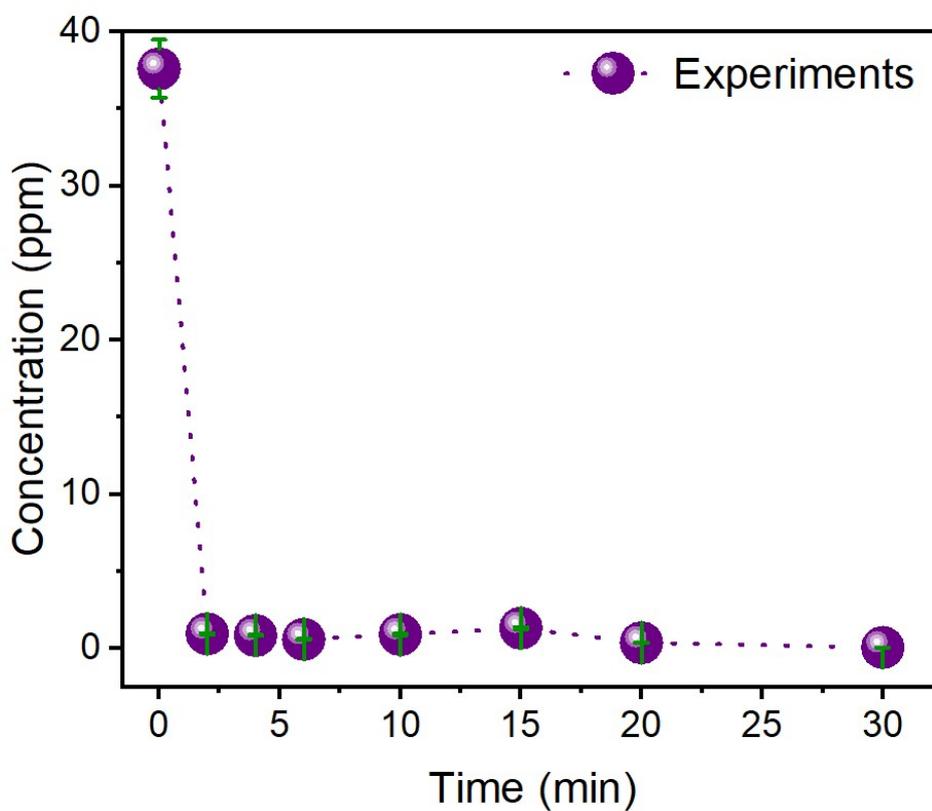


Figure S5:  $\text{MnO}_4^-$  kinetics plot of iPOP-6 (Conc. Vs Time curve)

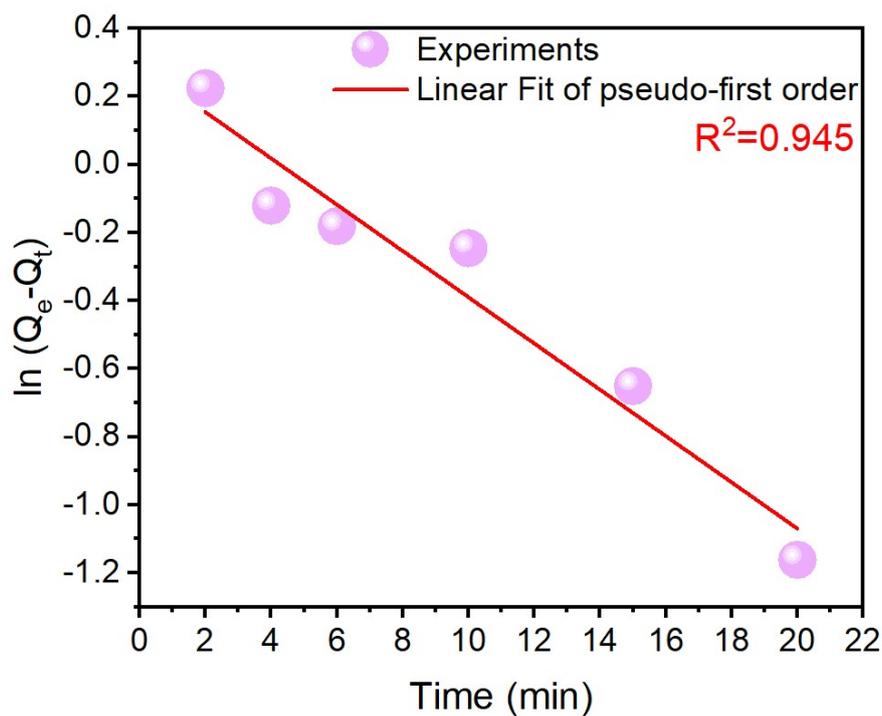


Figure S6: Pseudo-first order kinetics plot for  $\text{MnO}_4^-$  of iPOP-6

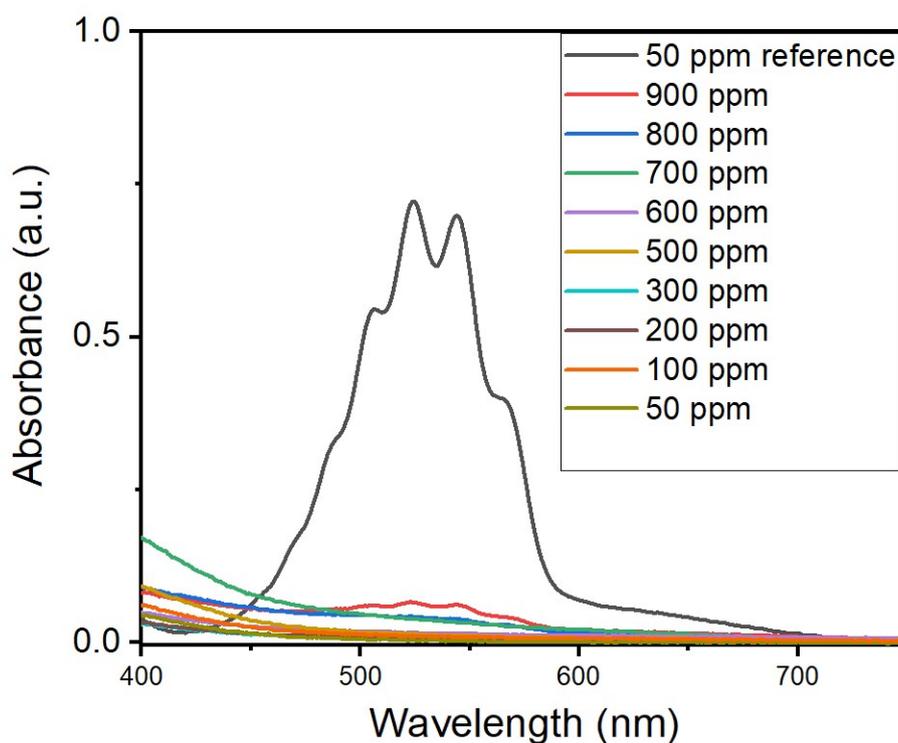
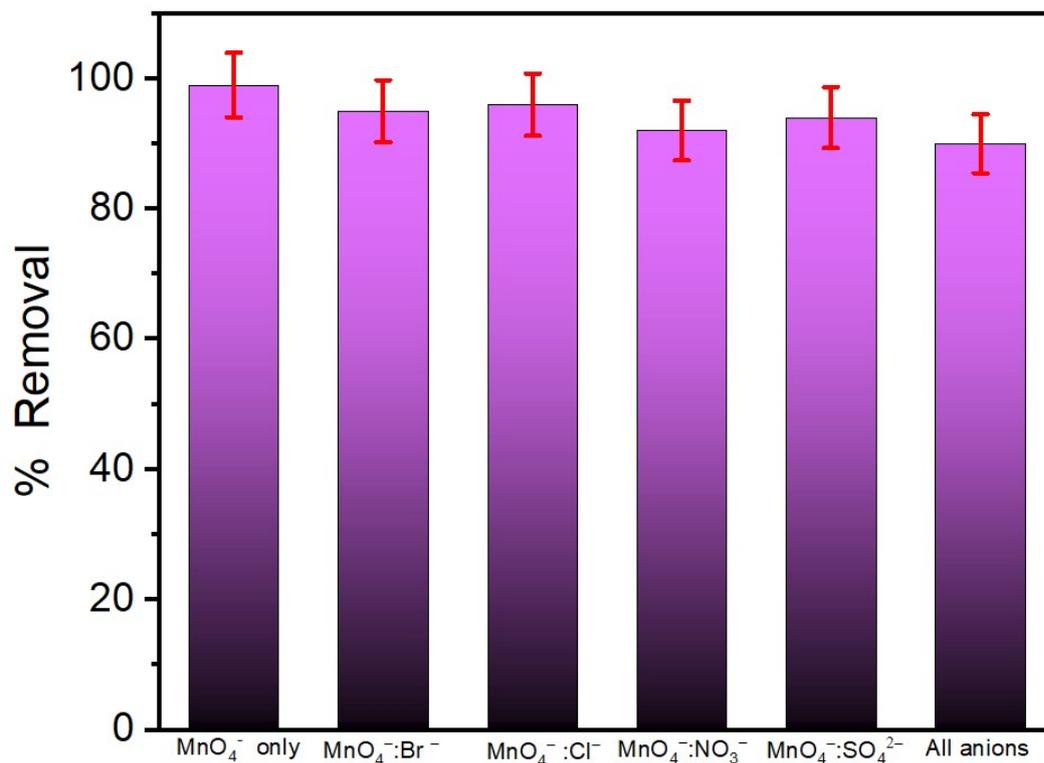
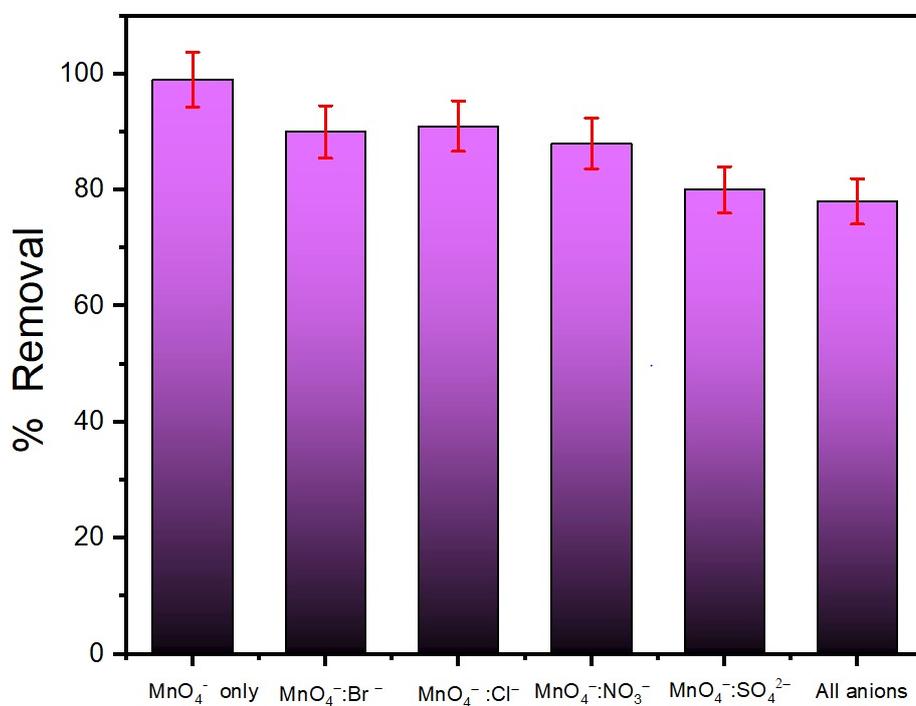


Figure S7: Residual absorbance of  $\text{MnO}_4^-$  after 6 hours with different concentration



**Figure S8: Removal of MnO<sub>4</sub><sup>-</sup> in presence of interfering ions (1:1)**



**Figure S9: Removal of MnO<sub>4</sub><sup>-</sup> in presence of interfering ions (1:10)**

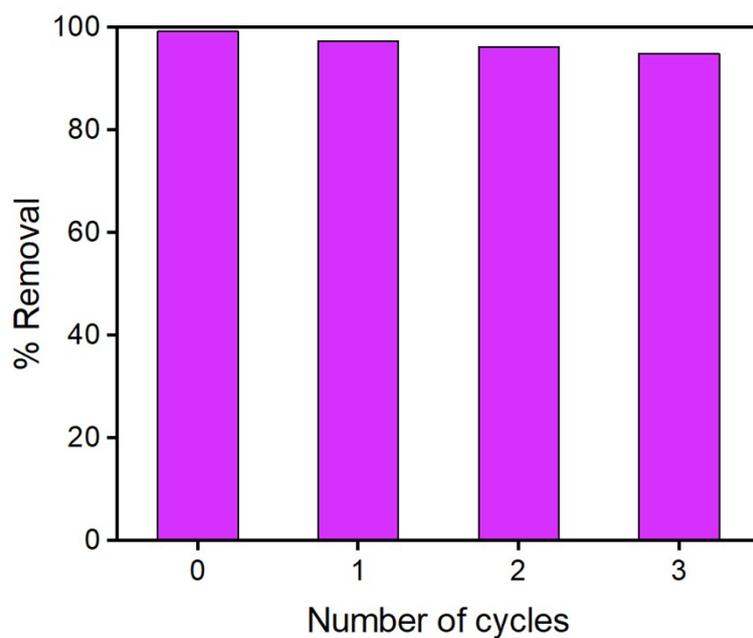


Figure S10: Recyclability experiments for  $\text{MnO}_4^-$

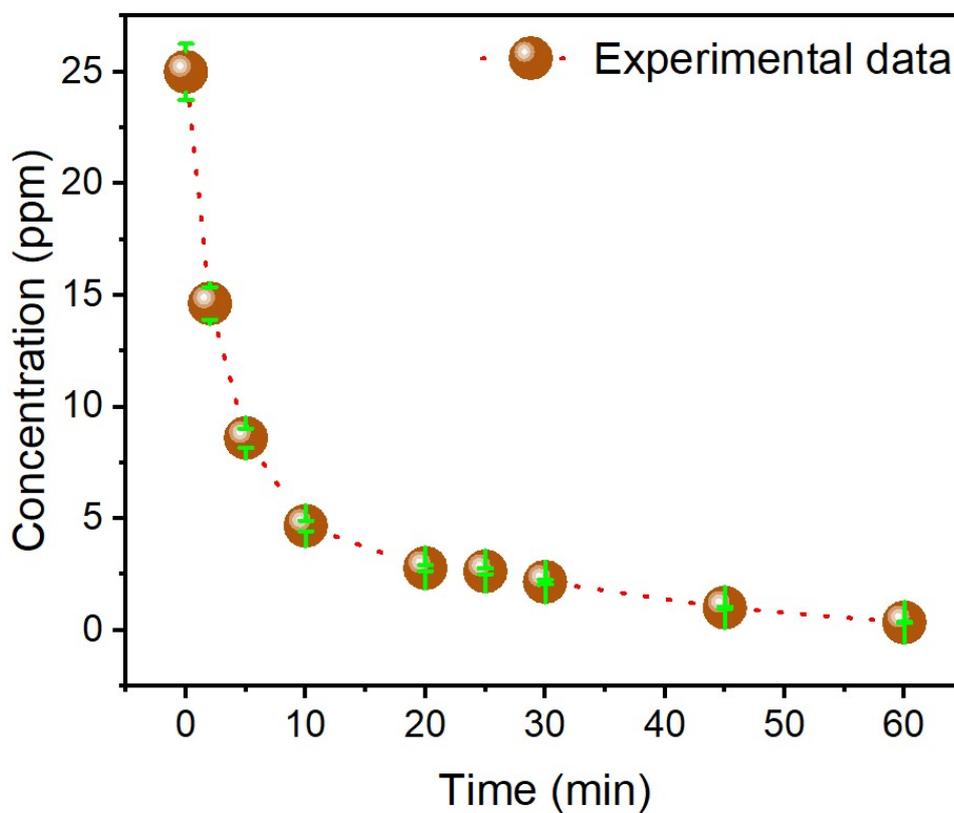


Figure S11:  $\text{I}_3^-$  kinetics plot of iPOP-6 (Conc. Vs Time curve)

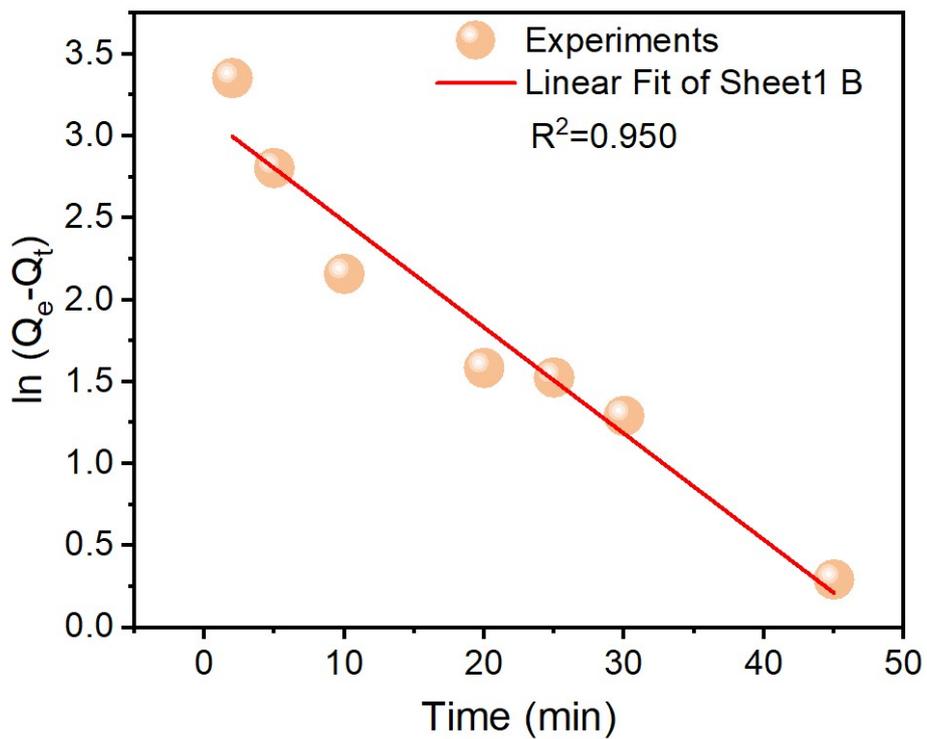


Figure S12: Pseudo-first order kinetics plot for  $I_3^-$  of iPOP-6.

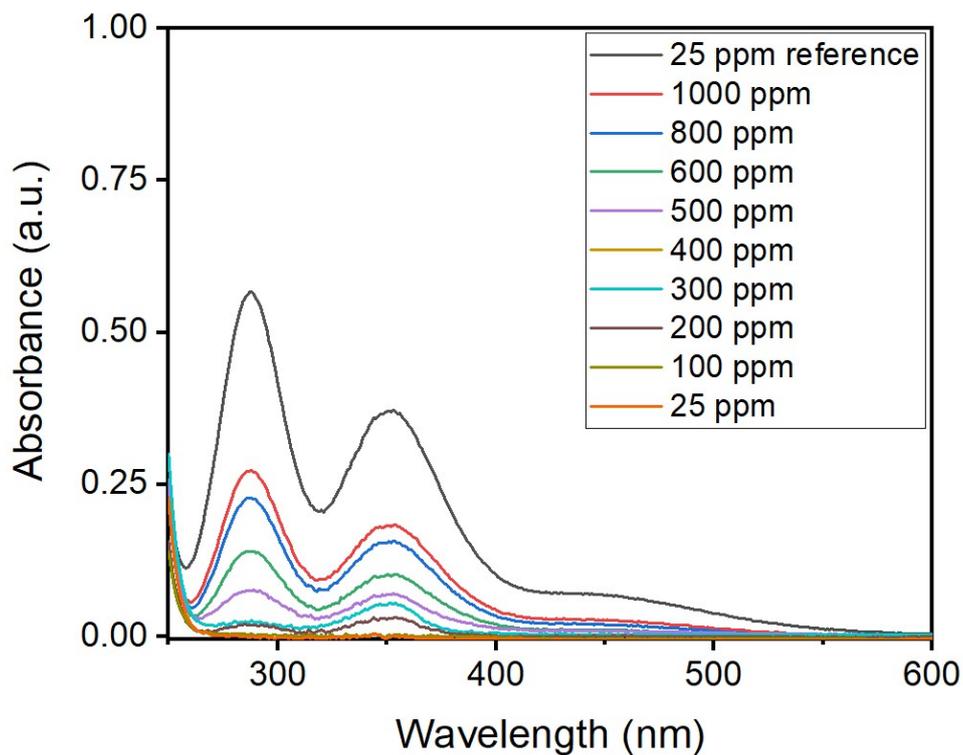
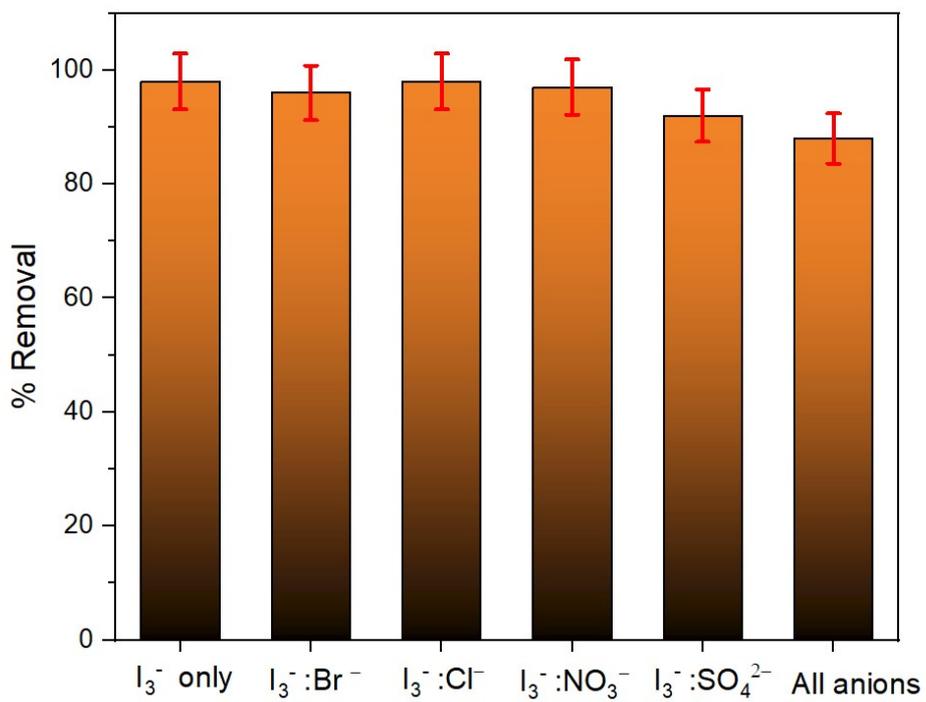
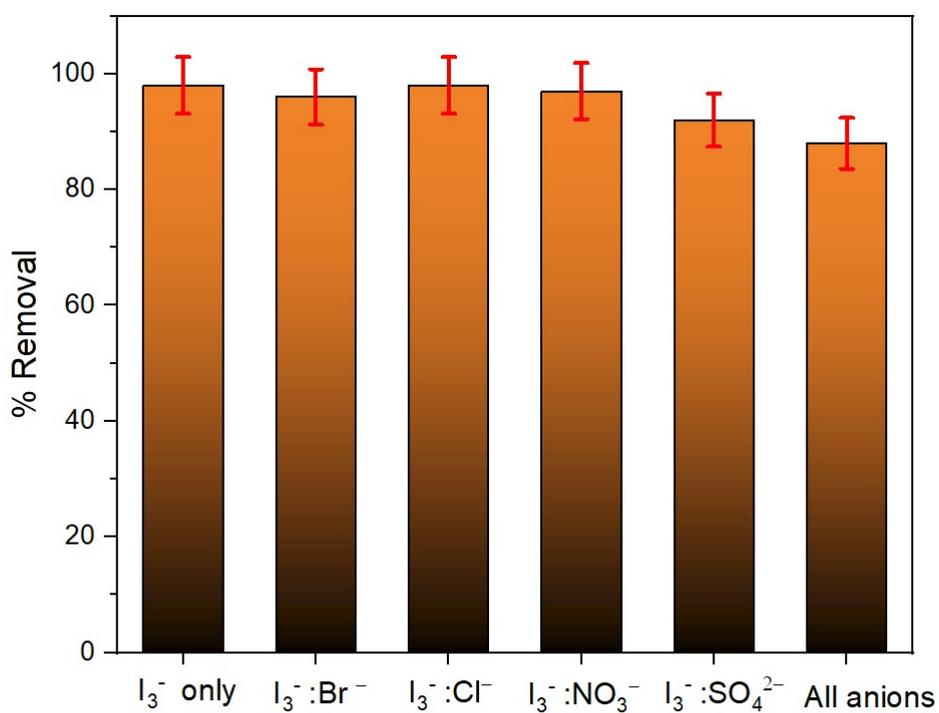


Figure S13: Residual absorbance of  $I_3^-$  after 6 hours with different concentration



**Figure S14: Removal of  $I_3^-$  in presence of interfering ions (1:1)**



**Figure S15: Removal of  $I_3^-$  in presence of interfering ions (1:10)**

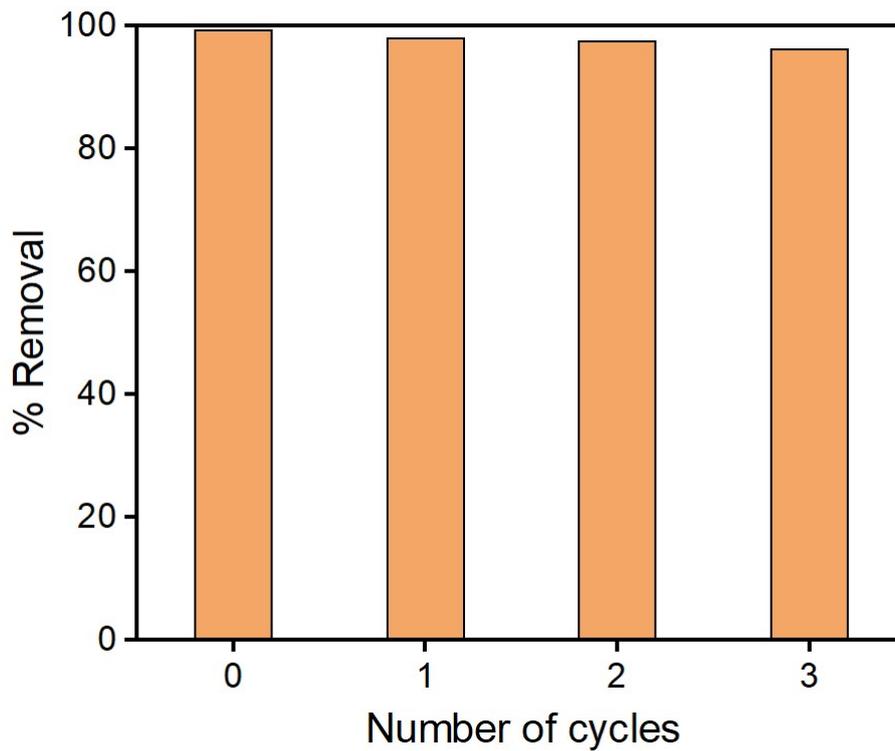


Figure S16: Recyclability experiments for  $I_3^-$

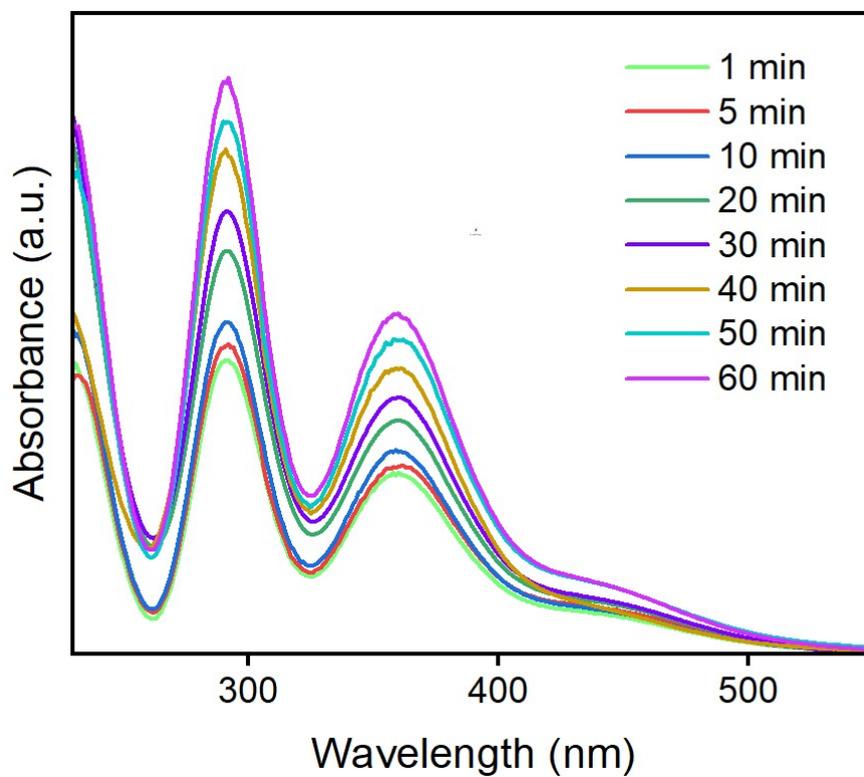


Figure S17: Iodine release in methanol from  $I_3^-@iPOP-6$

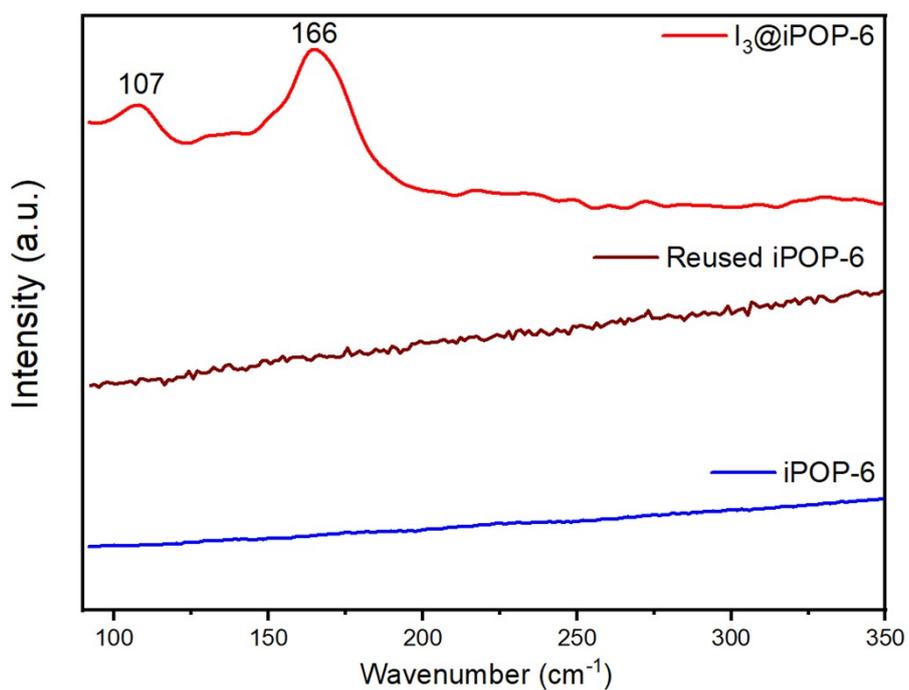


Figure S18: Post capture Raman spectra of  $I_3^-@iPOP-6$

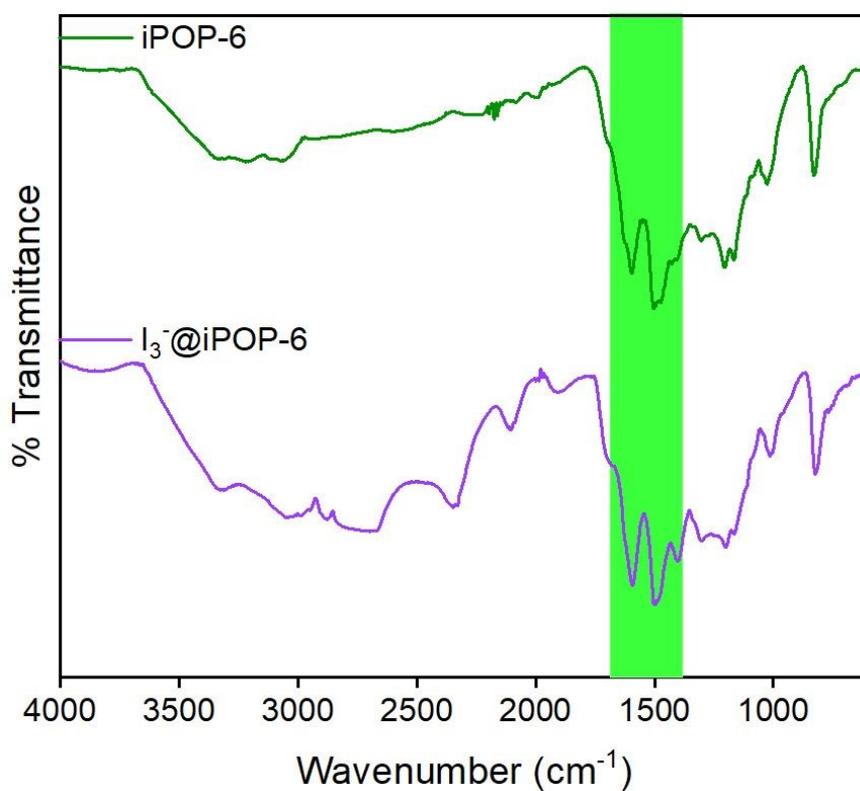


Figure S19: Post capture FT-IR spectra of  $I_3^-@iPOP-6$

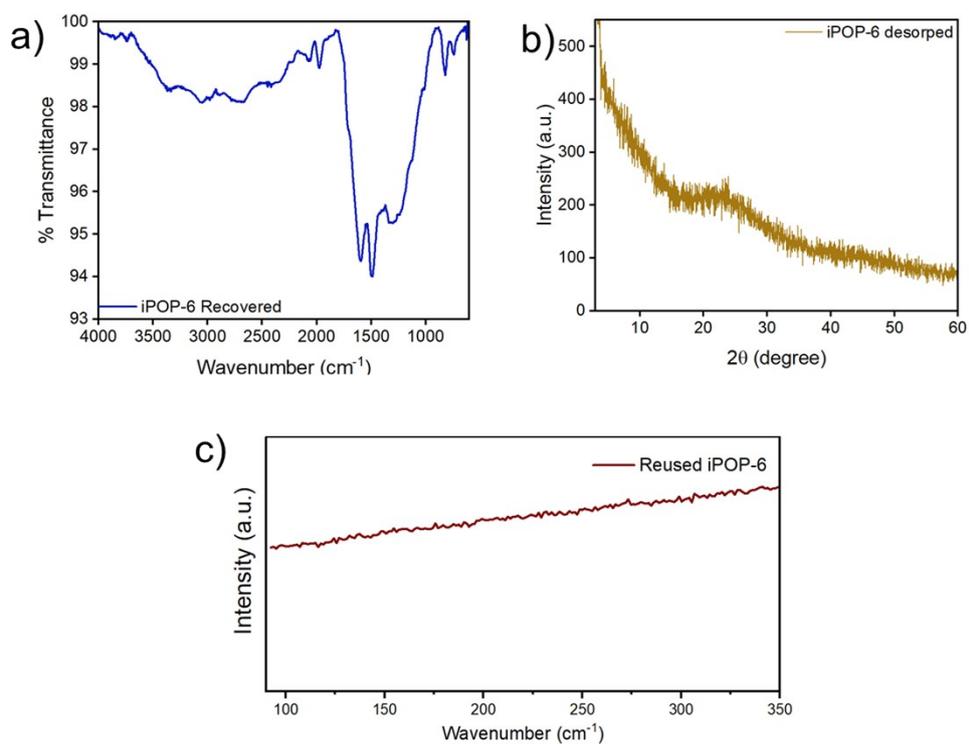


Figure S20: (a) FT-IR spectrum of the recovered iPOP-6; (b) PXRD patterns of the recovered iPOP-6 (c) Raman spectrum of the recovered iPOP-6.

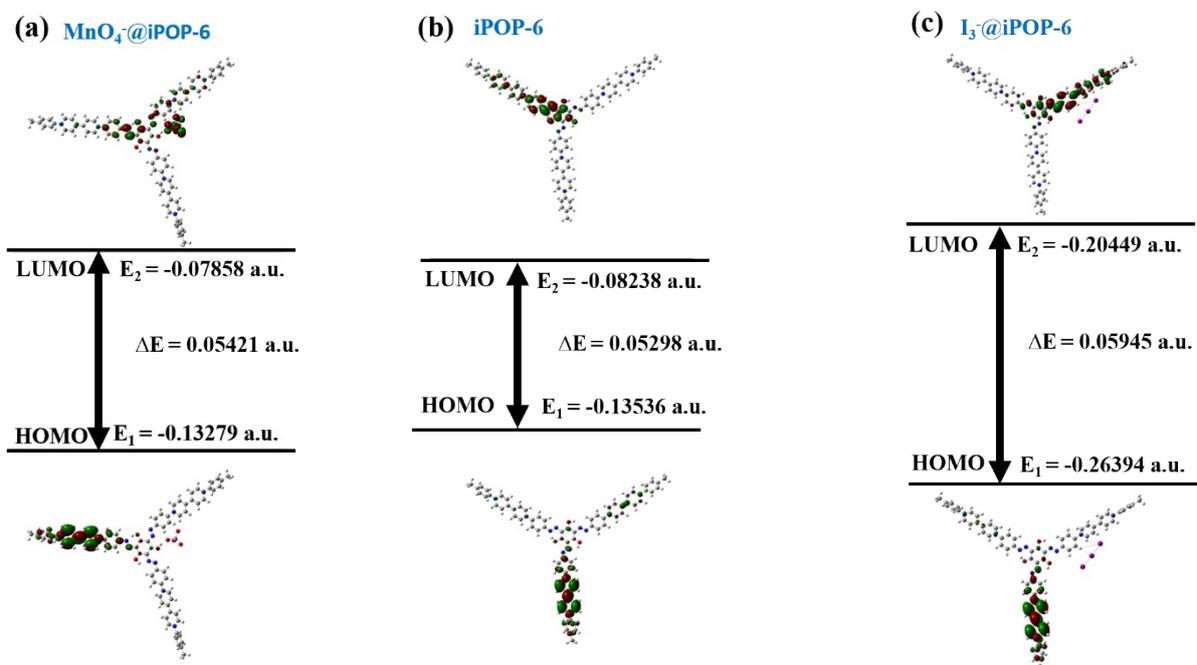


Figure S21: HOMO and LUMO of the adsorbate and complexes

**Table S1: Comparison table [N.D.-Not Done]**

Analyte	Name of the Adsorbate	Capacity(mg/g)	Selectivity	Reference
$\text{MnO}_4^-$	iPOP-6	854	$\text{Cl}^-$ , $\text{NO}_3^-$ , $\text{Br}^-$ , $\text{SO}_4^{2-}$	<b>This work</b>
$\text{I}_3^-$	iPOP-6	1021	$\text{Cl}^-$ , $\text{NO}_3^-$ , $\text{Br}^-$ , $\text{SO}_4^{2-}$	<b>This work</b>
$\text{MnO}_4^-$	SLUG-21	283	$\text{NO}_3^-$ , $\text{CO}_3^{2-}$	<i>J. Am. Chem. Soc.</i> , <b>2010</b> , 132, 7202-7209.
$\text{MnO}_4^-$	SCNU-Z1-C1	313.5	N.D.	<i>Inorg. Chem.</i> <b>2019</b> , 58, 4, 2899–2909
$\text{MnO}_4^-$	QUST-iPOP-1	517.7	$\text{Cl}^-$ , $\text{NO}_3^-$ , $\text{Br}^-$ , $\text{SO}_4^{2-}$	<i>ACS Appl. Mater. Interfaces</i> <b>2021</b> , 13, 33, 39404–39413
$\text{MnO}_4^-$	Compound-1	297.3	$\text{Cl}^-$ , $\text{NO}_3^-$ , $\text{Br}^-$ , $\text{SO}_4^{2-}$	<i>Chem.Sci.</i> <b>2018</b> , 9, 7874-7881
$\text{MnO}_4^-$	$\text{Ag}(\text{btr}) \cdot \text{PF}_6 \cdot 0.5\text{CH}_3\text{CN}$	163	$\text{NO}_3^-$ , $\text{BF}_4^-$ , $\text{ClO}_4^-$	<i>Inorg. Chem.</i> <b>2014</b> , 53, 12127-12134
$\text{MnO}_4^-$	IPcomp-6	281	$\text{Cl}^-$ , $\text{Br}^-$ $\text{NO}_3^-$ , $\text{ClO}_4^-$	<i>Angew. Chem. Int. Ed.</i> <b>2022</b> , 61, e2022033
$\text{MnO}_4^-$	Amberlite IR-120	4.9	N.D.	<i>Egypt. J. Aquat. Res.</i> <b>2015</b> 41, 2, 155–164
$\text{I}_3^-$	$\text{H}_2\text{C}(\text{OH})_2$ -7	1390	N.D.	<i>Angew. Chem. Int. Ed.</i> <b>2022</b> , 61, e2022141
$\text{I}_3^-$	Cadmium(II)-triazole MOF	180	N.D.	<i>Chem. Commun.</i> <b>2011</b> , 47, 7185-7187
$\text{I}_3^-$	MBM - MOF	880	N.D.	<i>Angew. Chem. Int. Ed.</i> <b>2018</b> , 57, 10148-10152.
$\text{I}_3^-$	THPS-C	926	N.D.	<i>Adv. Mater. Inter.</i> , <b>2019</b> , 6, 1900249
$\text{I}_3^-$	TNHCP2	850	N.D.	<i>Sep. Purif. Technol.</i> <b>2021</b> , 257, 117923
$\text{I}_3^-$	TAPB-BPDA COF	988.17	N.D.	<i>React. Funct. Polym.</i> , <b>159</b> (2021) 104806
$\text{I}_3^-$	PVDF/ZIF-8	73.33	N.D.	<i>Sep. Purif. Technol.</i> , <b>238</b> (2020) 116488
$\text{I}_3^-$	NTP	429	N.D.	<i>ACS Macro Lett.</i> , <b>2016</b> , 5, 1039