

## One-pot *in-situ* synthesis of NS-ligand codoped metal-organic framework for enhanced adsorption-assisted photocatalytic decontamination of antibiotics

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### Supporting Information

#### S1.

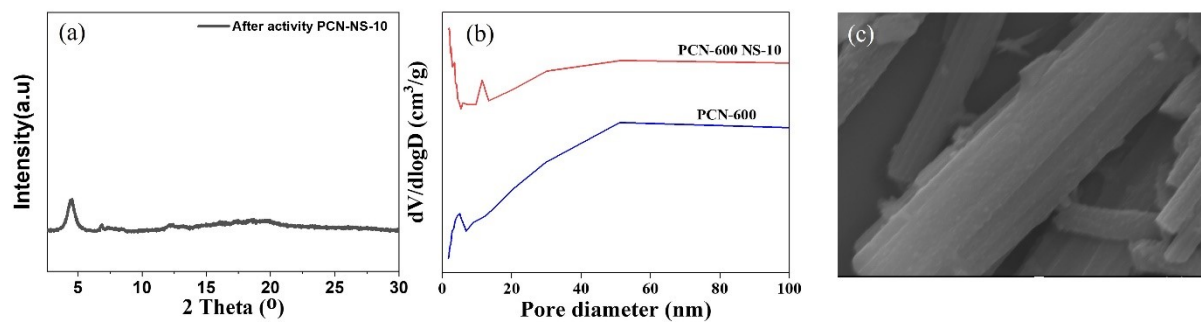
##### 3.1 Materials

All the reagents and raw materials were commercially purchased and employed in their original form without further modifications. Deionized water, produced from a deionized water plant with a resistivity of 18.25 MΩ·cm, prepared several solutions.  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  (99.9%), Tetrakis(4-carboxyphenyl)porphyrin (TCPP), 1,2-benzisothiazole-3-one (98%), Triethanolamine (98%) and Trifluoroacetic acid (99%), Isopropanol (99.5%), and Dimethylformamide (DMF) were obtained from Macklin

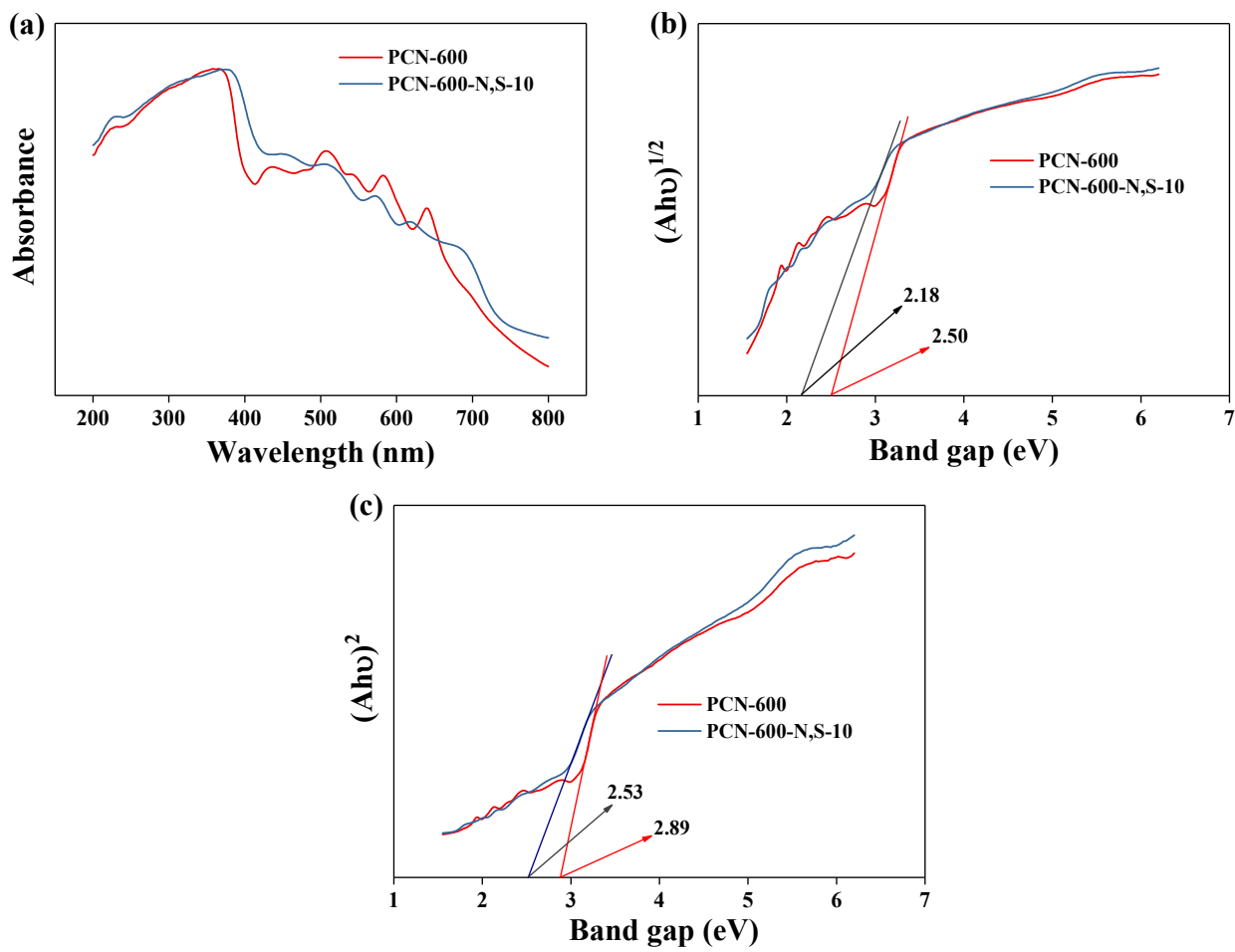
Chemical Reagent Co., Ltd. 5,5-Dimethyl-1-pyrroline N-oxide (DMPO, C<sub>6</sub>H<sub>11</sub>NO, 97%), and 2,2,6,6-Tetramethyl-4-piperidinol (TEMP, C<sub>9</sub>H<sub>19</sub>NO, >98%) were obtained from Aladdin Industrial Co. Ltd., China. Ethanol (C<sub>2</sub>H<sub>5</sub>OH, water ≤0.2%), p-benzoquinone (C<sub>6</sub>H<sub>4</sub>O<sub>2</sub>, 99%), and Metronidazole (99%) were acquired from Sinopharm Chemical Reagent Co., Ltd.

## S2

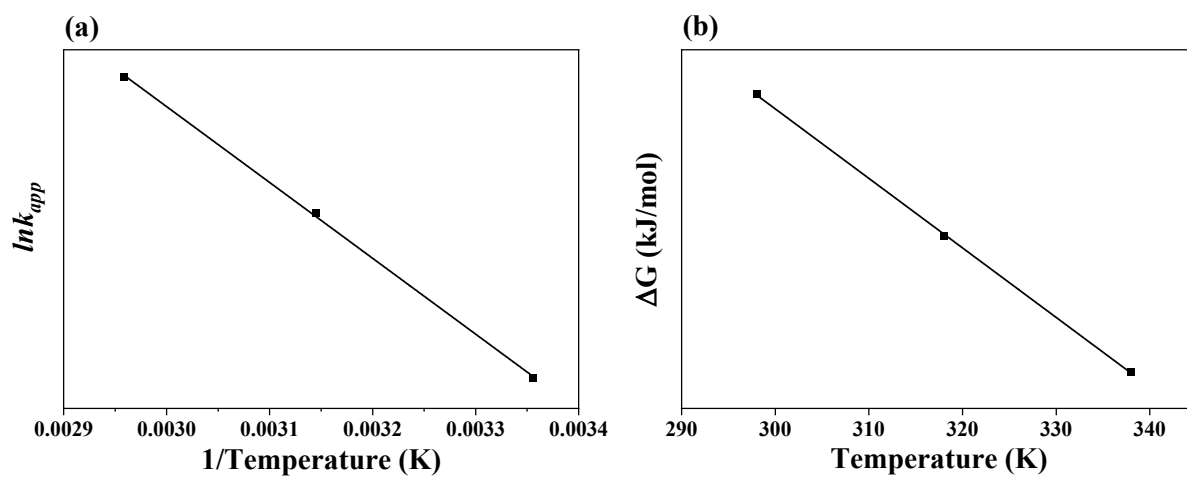
**3.5** The Fourier transform infrared (FT-IR) spectroscopy analyzed the functionality of PCN-600, PCN-600-NS-10, and PCN-600-NS-20 in the 400–4000 cm<sup>-1</sup> range conducted on a Thermo Nicolet Nexus 870 FT-IR spectrometer system (Nicolet, USA). The PXRD patterns were analyzed using a D/MAX-RB X-ray diffractometer (Rigaku, Japan) fitted with a Cu-K $\alpha$  radiation source operating at 40 kV and 40 mA. The Scanning Electron Microscope (SEM) (Zeiss, Germany) was used to investigate the morphology of PCN-600 at an operating voltage of 15 kV. The chemical composition and oxidation state were analyzed using X-ray photoelectron spectroscopy (XPS) using AlK $\alpha$  radiation, using equipment from Thermo Scientific in the United Kingdom. The nitrogen adsorption-desorption isotherms were conducted at a temperature of -196 °C using the Autosorb-1MP instrument manufactured by Quantachrome in the United States. The UV-vis spectrophotometer, specifically the SHIMADZU UV-2600 model, was employed to ascertain the band gap of the samples. Additionally, the Malvern Zetasizer, manufactured by Malvern Instruments Ltd in Malvern, UK, was utilized to establish the pH of the samples at the point of zero charge (pH<sub>pzc</sub>). The pH of the solutions was determined by employing a pH meter (METTLER TOLEDO Co. Ltd) coupled with a combined glass calomel electrode.



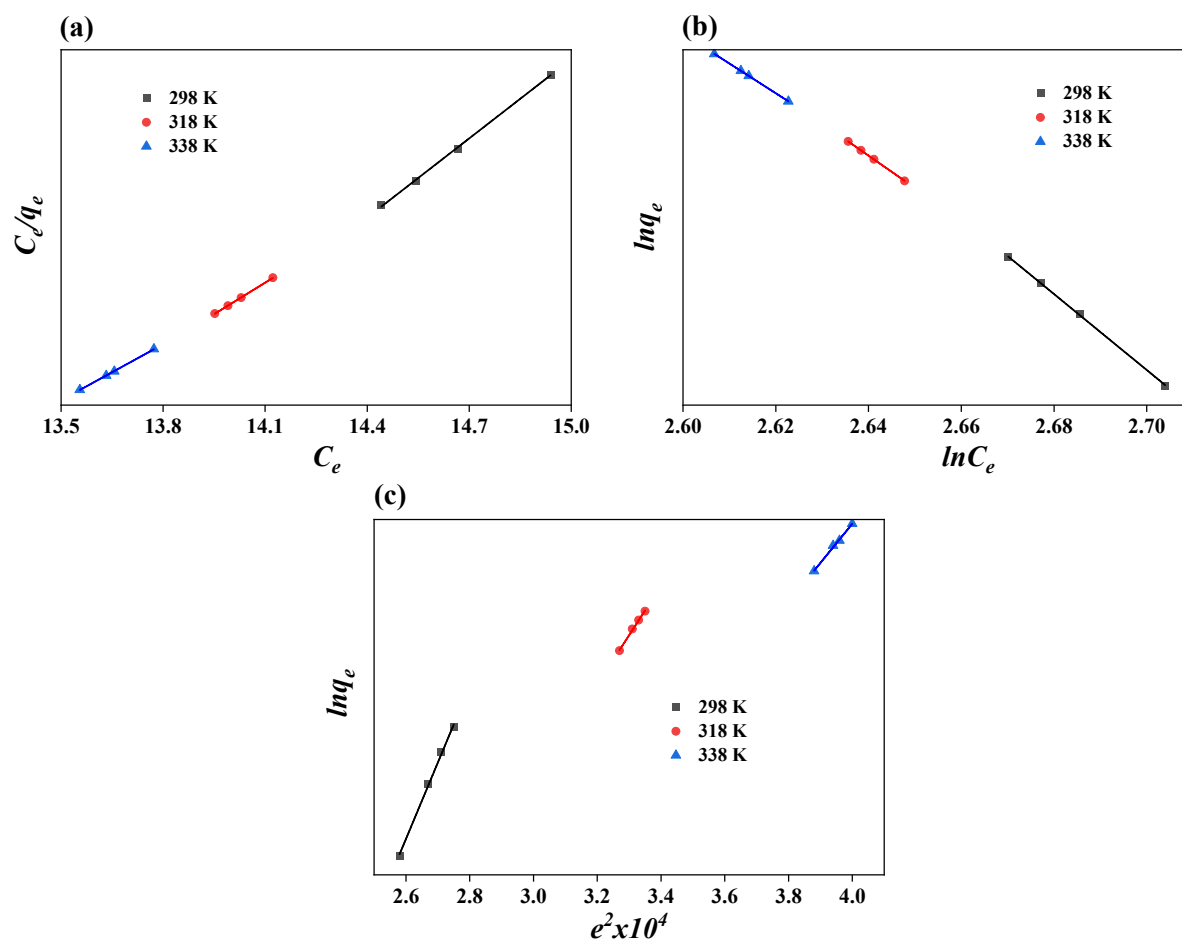
**Fig. S1**(a) Xrd after activity, b) Pore size distribution analysis using the Barret-Joyner-Halenda (BJH) method, and c) SEM after activity



**Fig. S2** UV-Visible spectra (a), Indirect band gap (b), and Direct band gap (c) of PCN-600 and PCN-600-N, S-10, respectively.



**Fig. S3** (a): Arrhenius plot showing  $\ln k_{app}$  vs  $1/T(K)$  for the determination of  $E_a$  values, and (b): Plot of Gibbs free energy change versus temperature.



**Fig. S4** Fitted profiles of (a) Langmuir, (b) Freundlich, and (c) DR adsorption isotherm, respectively, of CV dye using PCN-600-N, S-10.

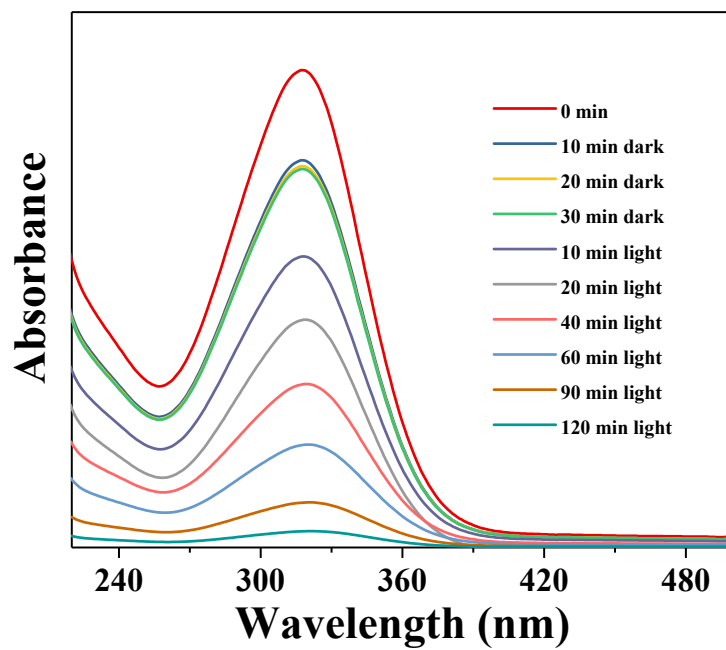
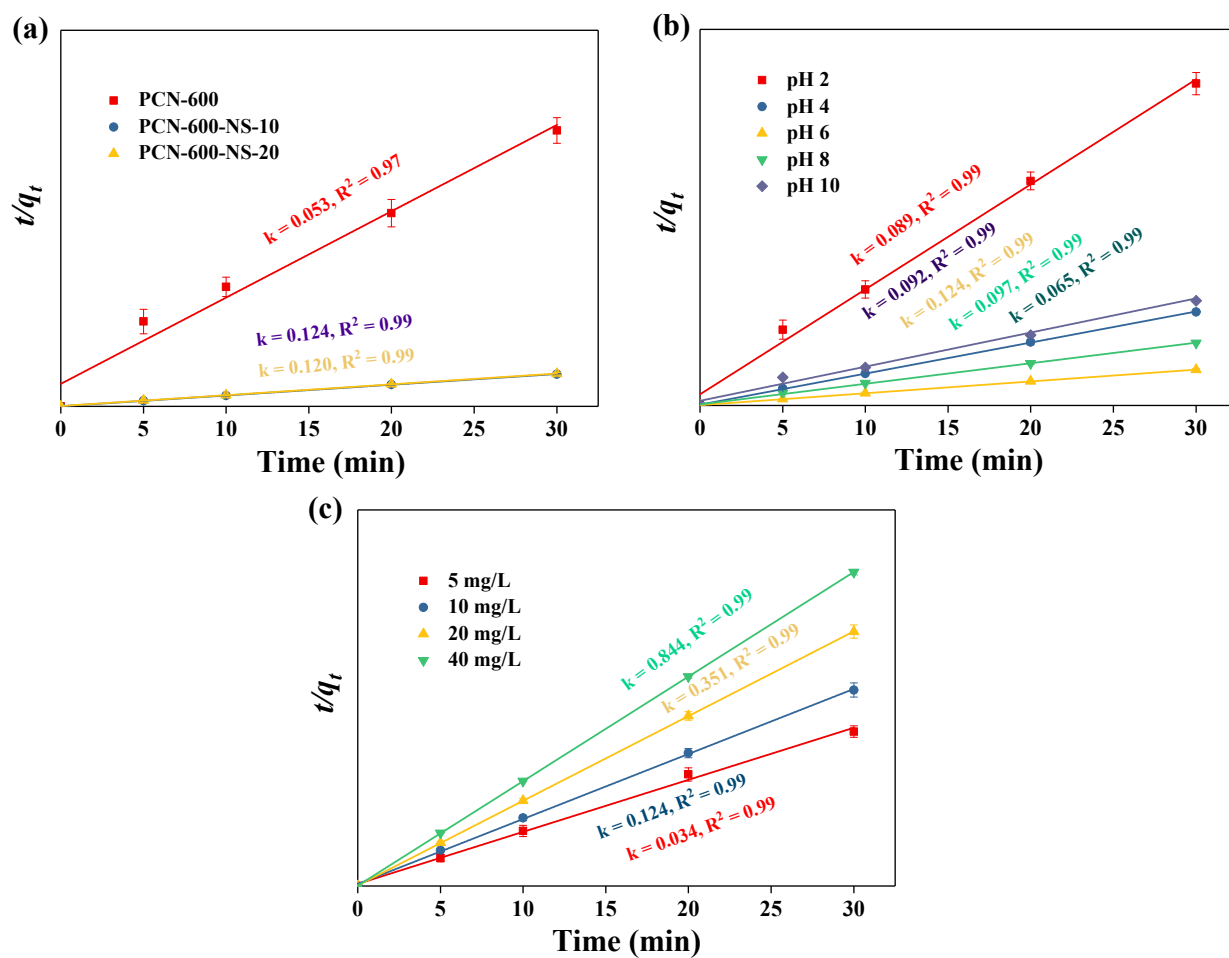
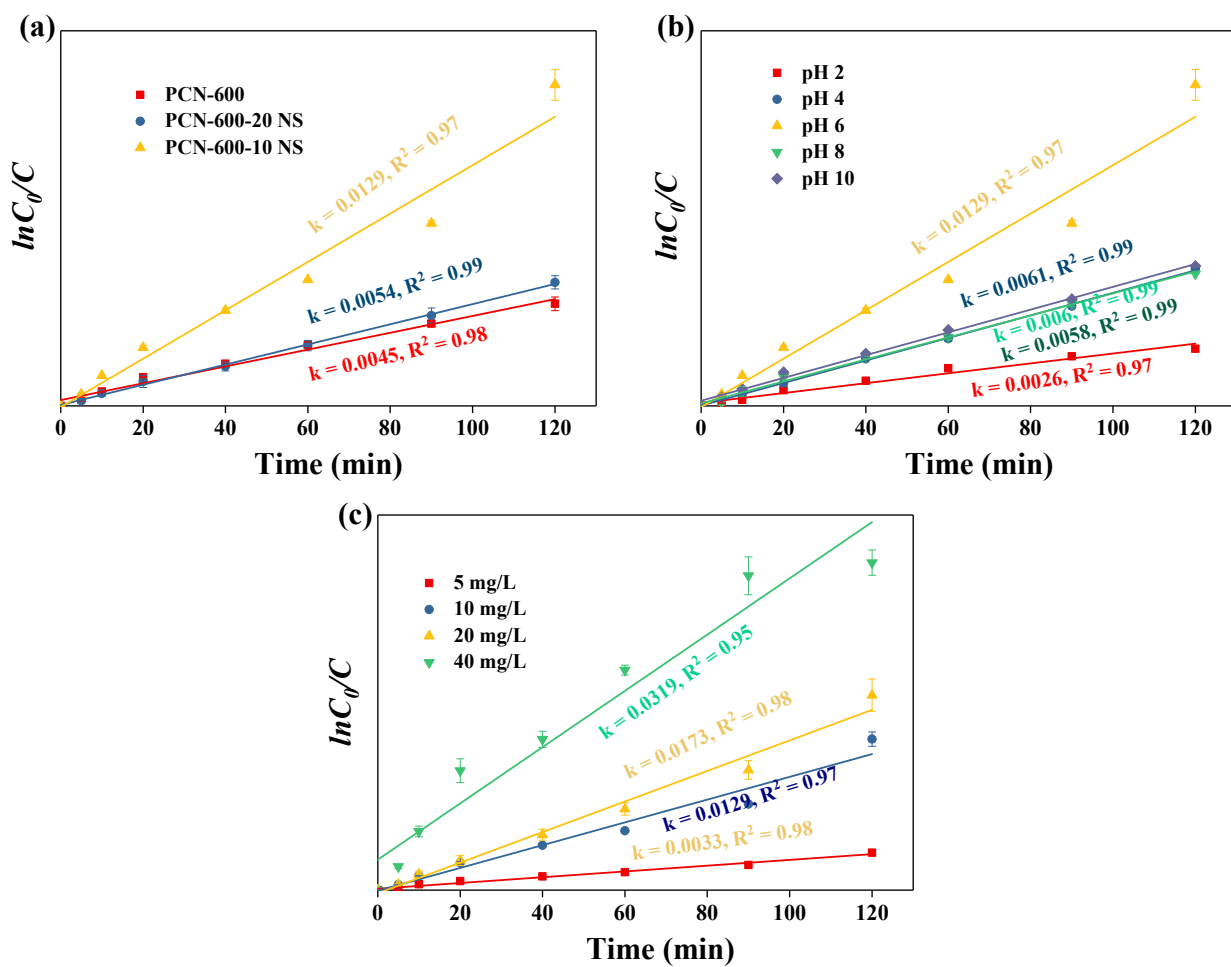


Fig. S5 UV-Visible spectra of MNZ at different time intervals during the removal process.

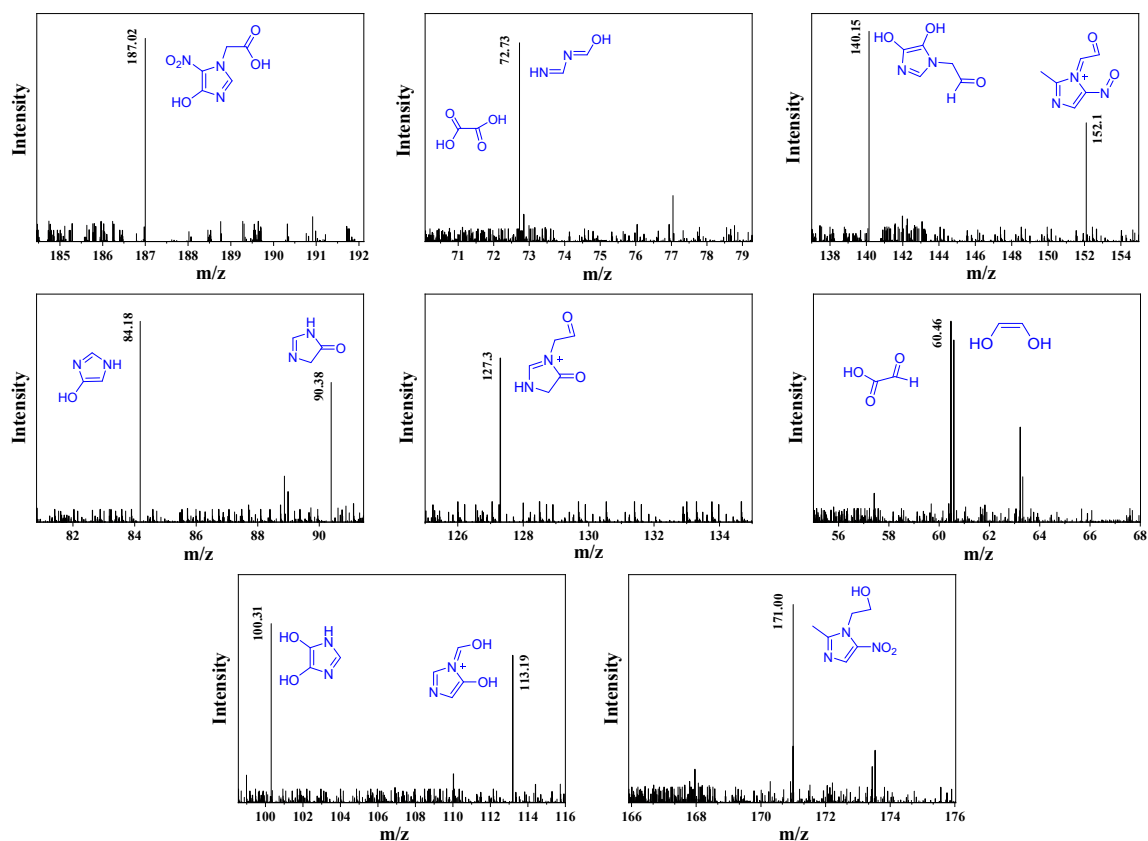


**Fig. S6** Pseudo-second order adsorption kinetics of MNZ using different catalysts (a), different initial solution pH (b), and different doses of PCN-600-NS-10 (c).





**Fig. S7** Pseudo-first order degradation kinetics of MNZ using different catalysts (a), different initial solution pH (b), and different doses of PCN-600-NS-10 (c).



**Fig. S8** Liquid-chromatography mass-spectrometry (LC-MS) spectra of metronidazole (MNZ) degradation.

**Table S1: Comparison of various catalytic systems for MTZ degradation.**

Catalyst	Adsorption capacity (mg/g)	MTZ concentration	Conditions	Degradation performance	Ref.
g-C <sub>3</sub> N <sub>4</sub> /LaFe <sub>0.5</sub> Cu <sub>0.5</sub> O <sub>3-δ</sub>	-	20 mg/L	[Catalyst] = 0.5 g/L, [H <sub>2</sub> O <sub>2</sub> ] = 0.3 mL/L, pH = 7.0, Vis-light	85% (150 min)	1
[Cu <sub>2</sub> (1,10-phenanthroline-5,6-dione) <sub>3</sub> (PMo <sub>12</sub> O <sub>40</sub> ) <sub>2</sub> ·3H <sub>2</sub> O	-	30 mg/L	[Catalyst] = 0.01 g/L, UV-light, pH <sub>0</sub> = 3.	80% (150 min)	2
CoFe <sub>2</sub> O <sub>4</sub> /RC	-	-	-	-	-
Fe <sub>3</sub> O <sub>4</sub> /rGO/TiO <sub>2</sub>	-	20 mg/L	[Catalyst] = 0.75 g/L, Vis-	96% (120 min)	3

mZVI@C-800	-	5 mg/L	light, T = 25 °C [Catalyst] = 0.25 g/L, [Sulfite] = 0.1 g/L, pH = 3, T = 25 °C	min) 81% (60 min)	4
Magnetic biochar	-	20 mg/L	[Catalyst] = 0.7 g/L, [PS] = 1.0 mM, pH <sub>0</sub> = 6.3	95 (180 min)	5
<b>PCN-600-NS-10</b>	<b>57.6</b>	<b>20 mg/L</b>	<b>[Catalyst] = 0.01 g/L, pH = 8.0, T = 25 °C).</b>	<b>87% (150min)</b>	<b>This study</b>

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## References

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