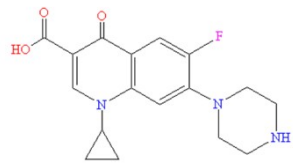
Supplementary Information

Degradation of ciprofloxacin by persulfate activated with pyrite: mechanism, acidification and tailwater reuse

1. Physicochemical properties of ciprofloxacin

Table S1 Physicochemical properties of ciprofloxacin

Antibiotic	Ciprofloxacin
Molecular formula	$C_{17}H_{18}FN_3O_3$
Molecular weight	332.1
Structural formula	
Relative density (water is 1 g/cm^3)	1.461 ± 0.06 g/cm^3
Solubility in water (25℃)	1.0 mg/mL
Acidity coefficient (pka)	4.04
Log *Kow* Syracuse [1]	0.28
Log *Kow* [2]	1.24 ± 0.86

[1]From http://esc.syrres.com/interkow/estsoft.htm

[2]Estimated with ACD Log P software(Advanced Chemica I Development, Toronto, Canada).

2. Basic physical and chemical properties of different water substrates

Table S2 Physicochemical properties of different water substrates

Physicochemical property	Tap water	River water
pH	7.75	7.96
TOC	44.68 mg/L	30.67 mg/L
Na^+	27.44 mg/L	140.02 mg/L
K^+	1.92 mg/L	15.18 mg/L
Ca^{2+}	77.125 mg/L	49.21 mg/L
Mg^{2+}	20.59 mg/L	29.56 mg/L
F^-	2.78 mg/L	2.88 mg/L
Cl^-	277.76 mg/L	318.40 mg/L
HCO_3^-	148.32 mg/L	152.50 mg/L
NO_3^-	16.45 mg/L	17.53 mg/L
SO_4^{2-}	104.91 mg/L	121.69 mg/L

Note: The river water was taken from the Wuma River, Taigu, Jinzhong City, Shanxi Province on November 30, 2021 (37°26’56’’ N, 112°33’53” E)

3. The removal of CIP by FeS_2 or PS

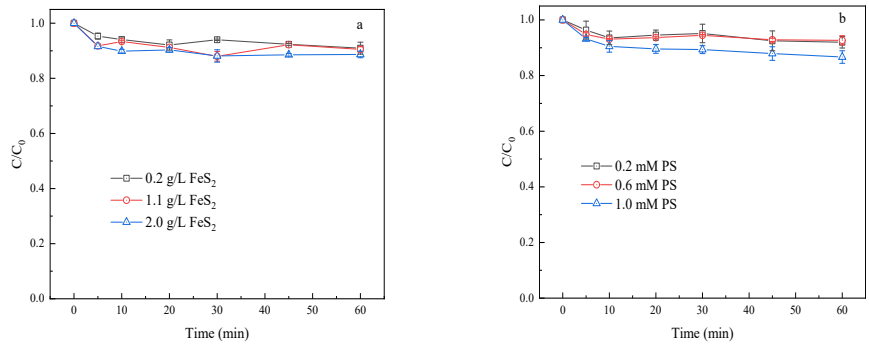


Fig. S1 The removal of CIP by FeS_2 (a) or PS (b)

([CIP]=30 μM)

4. Ultraviolet and visible spectra of ciprofloxacin before and after FeS_2/PS processes

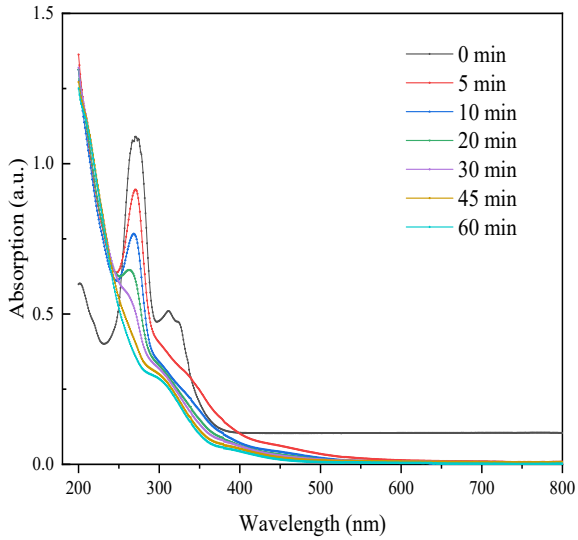


Fig. S2 Ultraviolet and visible spectra of ciprofloxacin before and after FeS_2/PS processes.

([CIP]=30 μM, [FeS_2]=2.0 g/L, [PS]=1 mM)

5. The pH before and after the reaction under different pH conditions

Table S3 The pH before and after the reaction under different pH conditions

([CIP]=30 μM, [FeS_2]=2.0 g/L, [PS]=1 mM)

Condition	pH=2	pH=4	pH=6	pH=8	pH=10	Control
Before	2.00	3.99	6.00	7.97	10.02	5.40
After	1.98	2.94	2.94	3.07	3.06	2.93

6. pH of the control at different reaction times

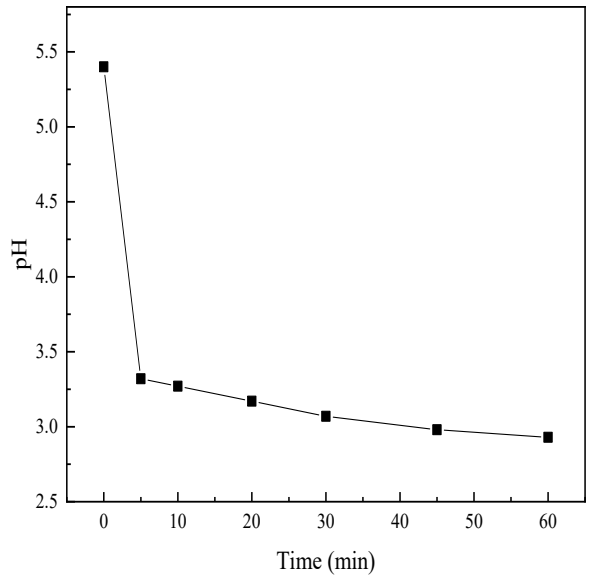


Fig. S3 pH of the control at different reaction times

([CIP]=30 μM, [FeS_2]=2.0 g/L, [PS]=1 mM)

7. SEM and EDS spectra of fresh and used pyrite

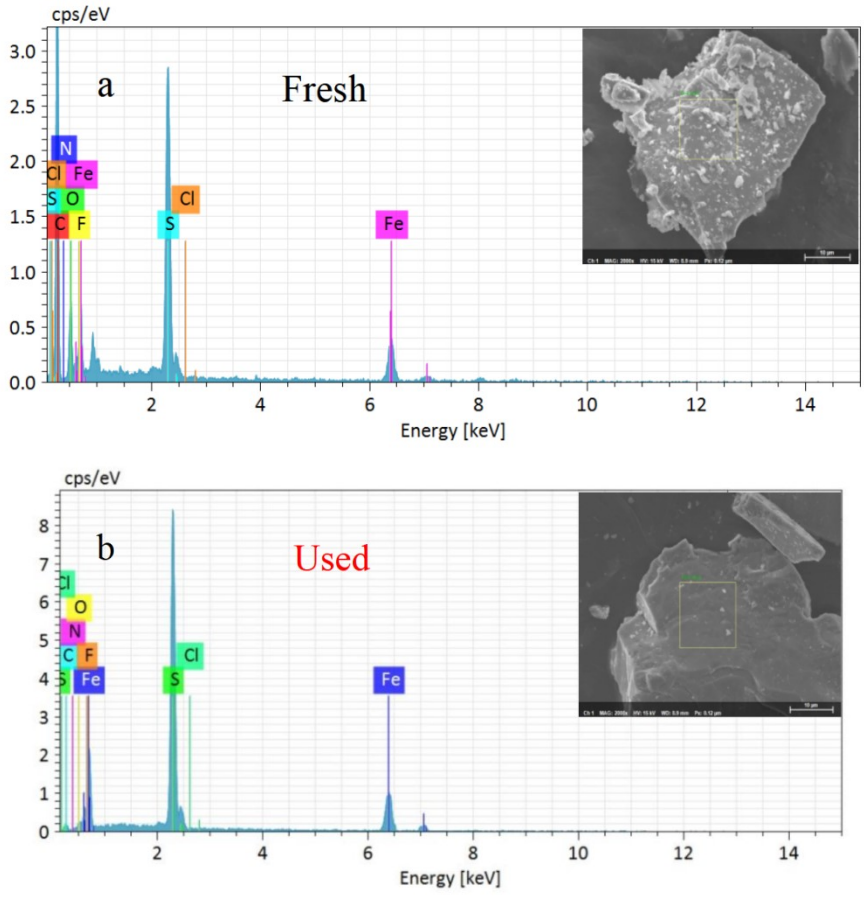


Fig. S4 SEM and EDS spectra of fresh (a) and used (b) pyrite

8. FTIR spectra of fresh and used pyrite

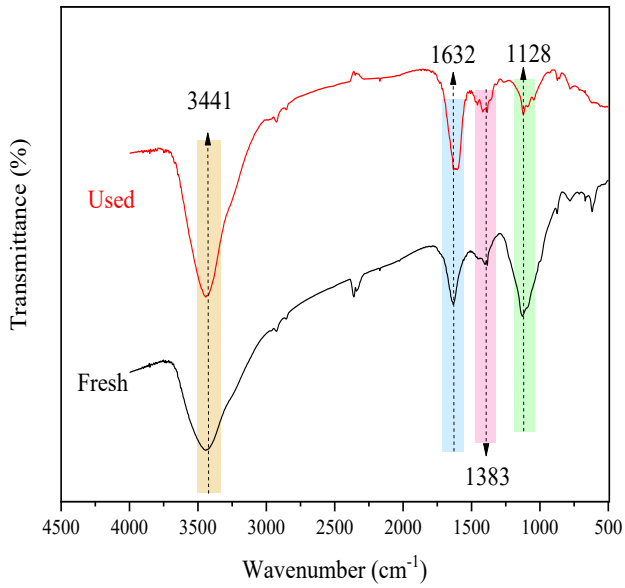


Fig. S5 FTIR spectra of fresh and used pyrite

9. Effect of different water substrates pH=4 on the degradation of CIP by FeS_2/PS

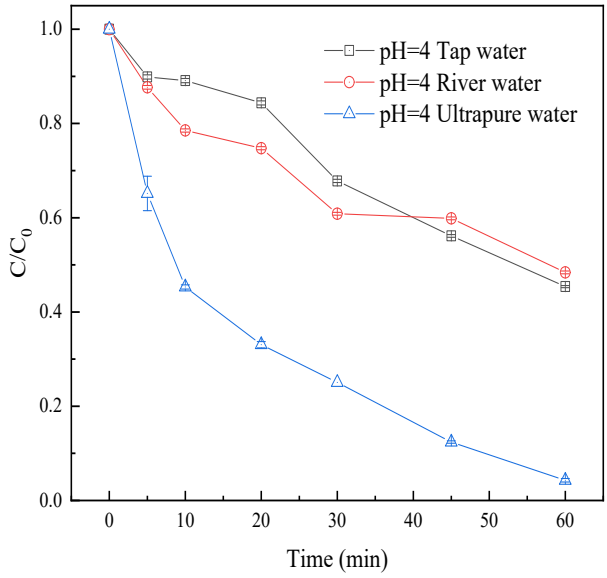


Fig. S6 Effect of different water substrates pH=4 on the degradation of CIP by FeS_2/PS ([CIP]=30 μM, [FeS_2]=2.0 g/L, [PS]=1 mM).

10. Analysis results of LC-MS (ESI-) degradation products

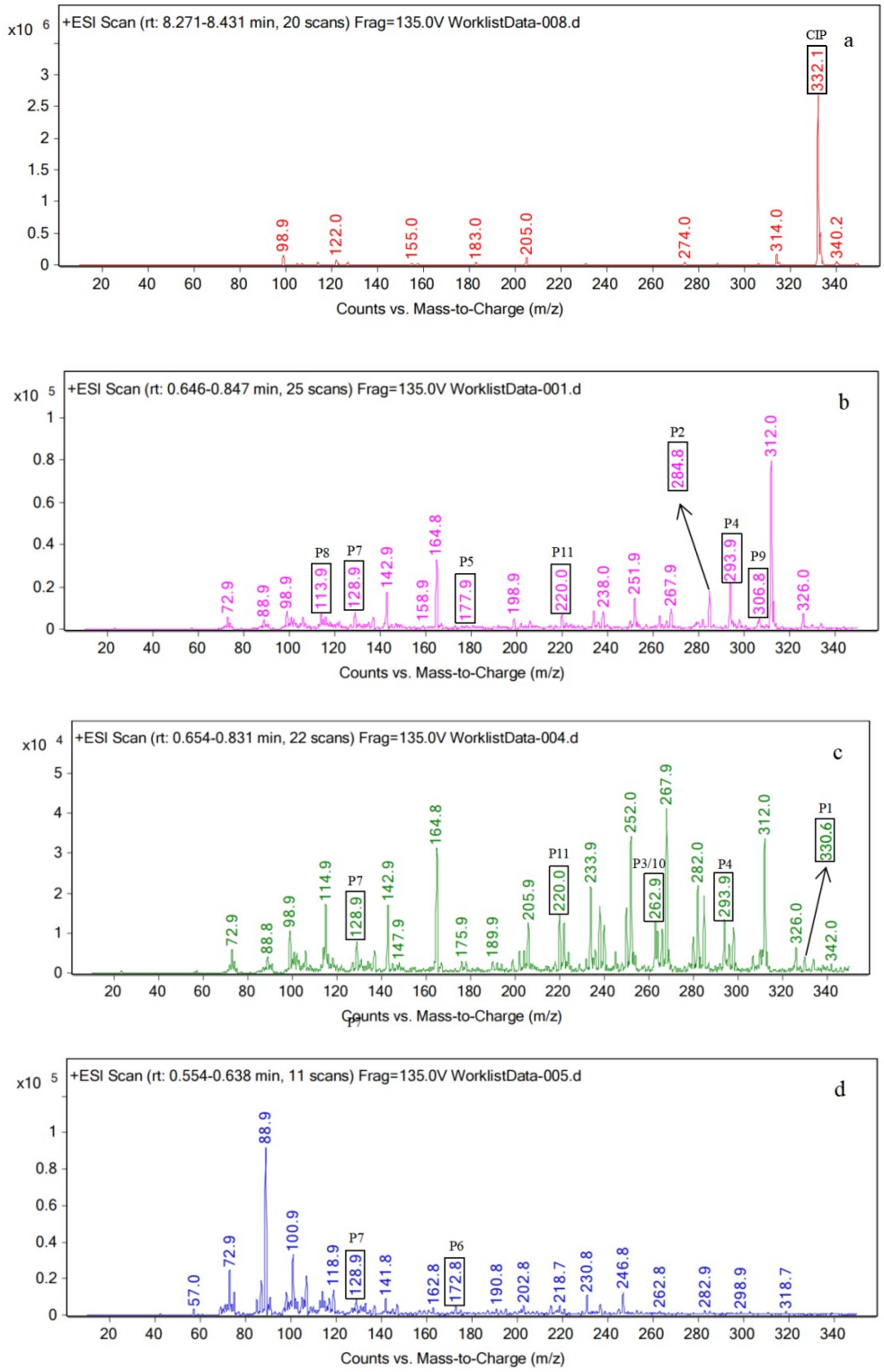
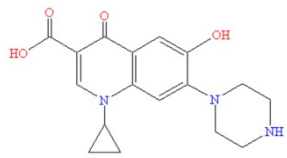
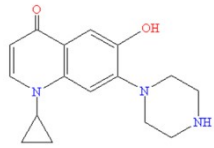
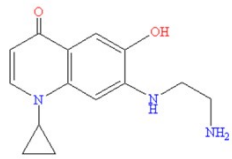
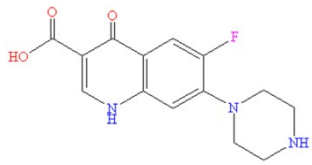
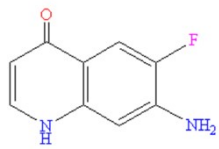
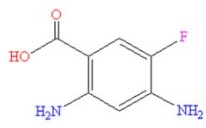
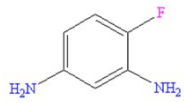
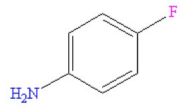
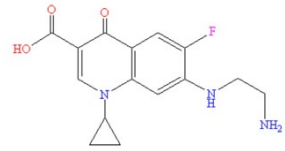
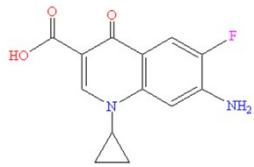
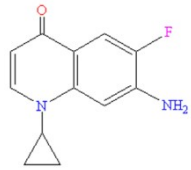


Fig. S7 Analysis results of LC-MS(ESI-) degradation products at 0 min(a), 15 min(b), 30 min(c), and 60 min(d).

11. Intermediates of CIP degradation by FeS_2/PS system

Table S4 Intermediates of CIP degradation by FeS_2/PS system

Products	*m/z*	Structural formula
CIP	332.1	
P1	330.1	
P2	285.2	
P3	260.1	
P4	292.1	
P5	178.1	
P6	170.1	
P7	127.1	

P8	112.1	
P9	306.1	
P10	263.1	
P11	219.1	

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