Supporting information

Highly Efficient Degradation of Sulfisoxazole by Natural Chalcopyrite-Activated Peroxymonosulfate: Reactive Species and Effects of Water Matrices

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Thirteen pages include 1 Note, 2 Tables, and 15 Figures.

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Note S1. Analysis of degradation products.

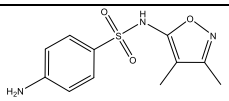
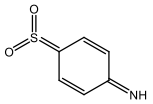
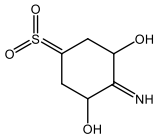
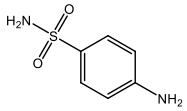
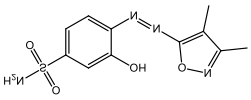
The degradation products of SIX were analyzed using a Waters Acquity ultra-performance liquid chromatograph (UPLC) H-class system with a Xevo G2-XS triple quadrupole mass spectrometer (MS/MS). An Acquity UPLC BEH Shield RP C18 column (2.1 × 150 mm, 1.7 μm) was used for the separation. The triple quadrupole MS was operated in a full-scan mode with positive electrospray ionization (ESI+) as the ion source and the capillary voltage was set at 2.5 kV. Nitrogen was used as the cone and desolvation gas. The full-scan MS spectra were recorded by scanning from an m/z of 40 to an m/z of 400.

Table S1. Elemental compositions of fresh and used chalcopyrite.

	Atomic %				
	Cu	Fe	S	C	O
Fresh chalcopyrite	10.0	9.9	21.8	31.8	26.5
Used chalcopyrite	4.0	9.6	11.5	39.0	35.9

Data source: XPS

Table S2. Intermediate products of SIX degradation in chalcopyrite-PMS oxidation.

Compound	R.T. (min)	m/z	Molecular formula	Proposed structure
SIX	3.84	268	$C_{11}H_{13}N_3O_3S$	
TP1	0.70	156	$C_6H_6NSO_2$	
TP2	0.93	192	$C_6H_8N_2O_2S$	
TP3	7.46	173	$C_6H_9NSO_4$	
TP4	12.2	297	$C_{11}H_{12}N_4SO_4$	

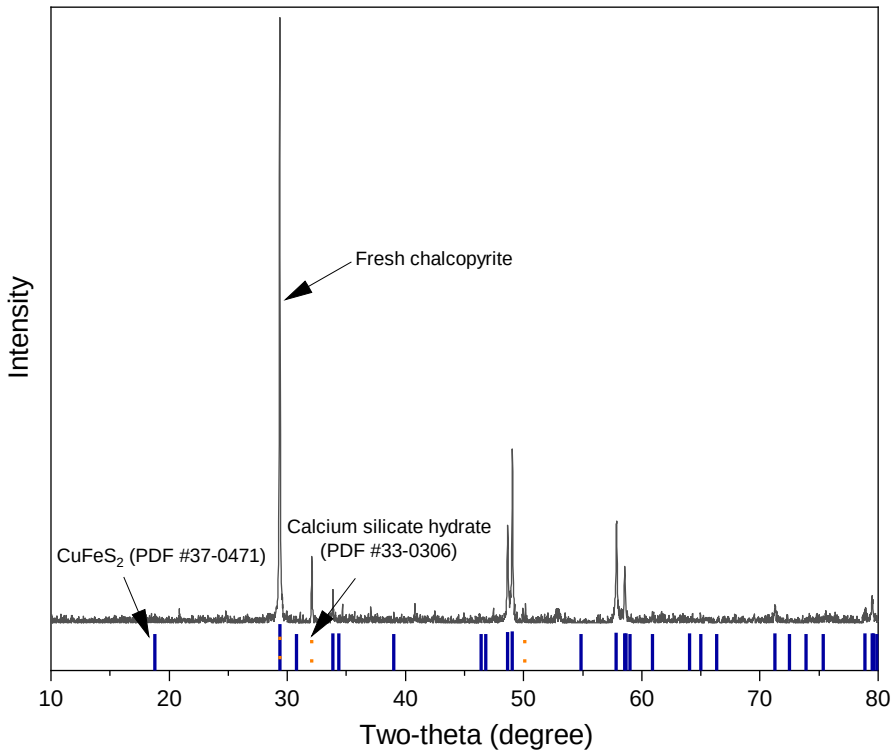


Figure S1. XRD pattern of fresh chalcopyrite.

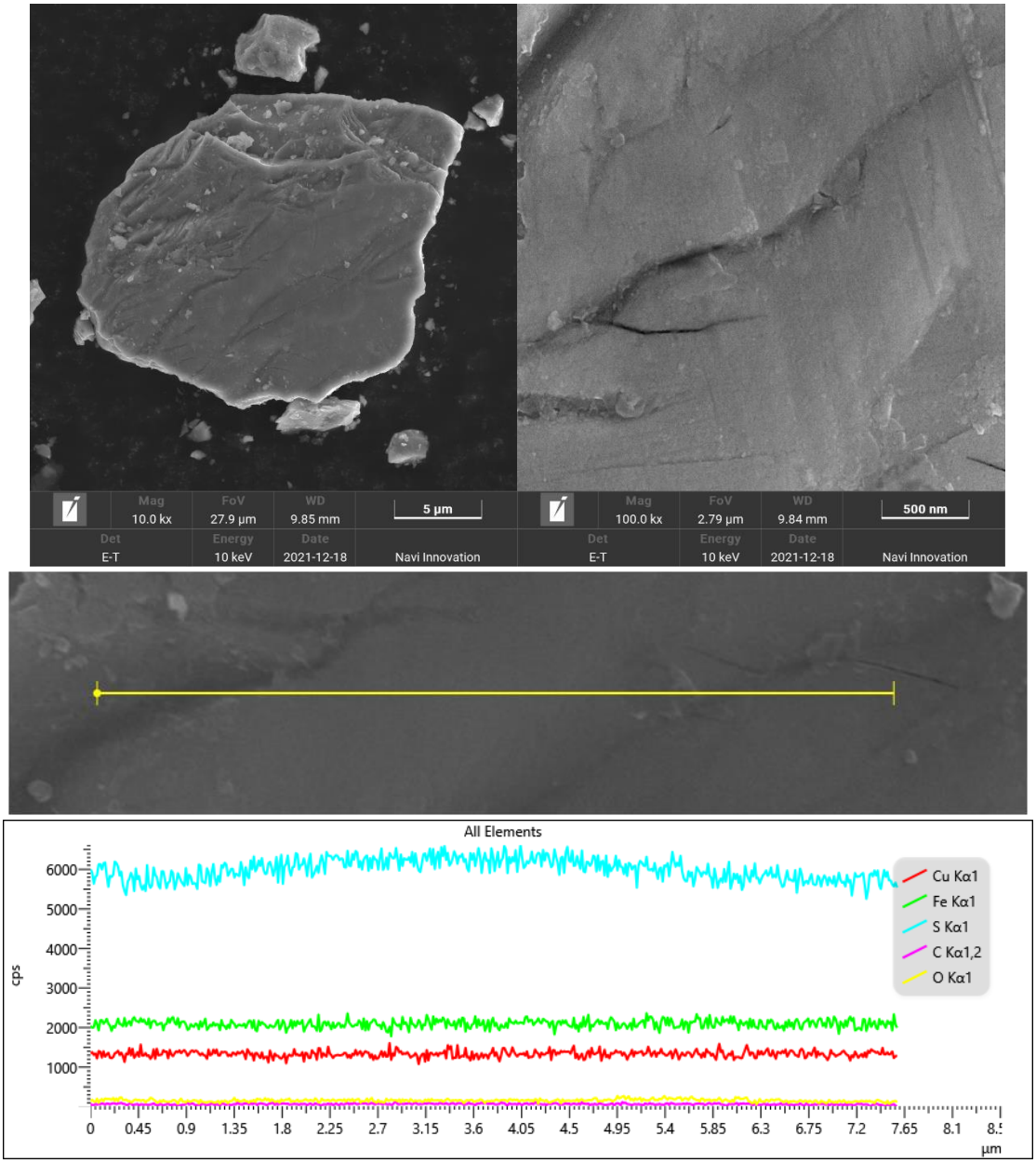


Figure S2. (a, b) SEM images of chalcopyrite with different magnifications and (c) EDS spectrum of chalcopyrite.

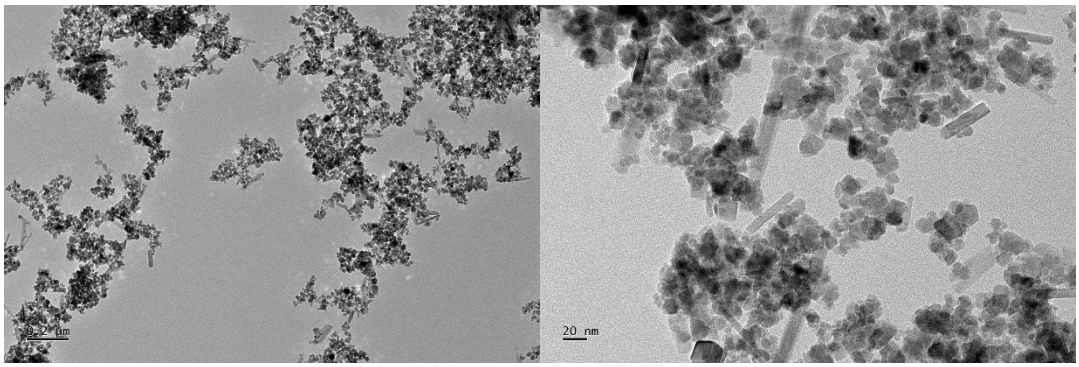


Figure S3. SEM images of magnetite with different magnifications.

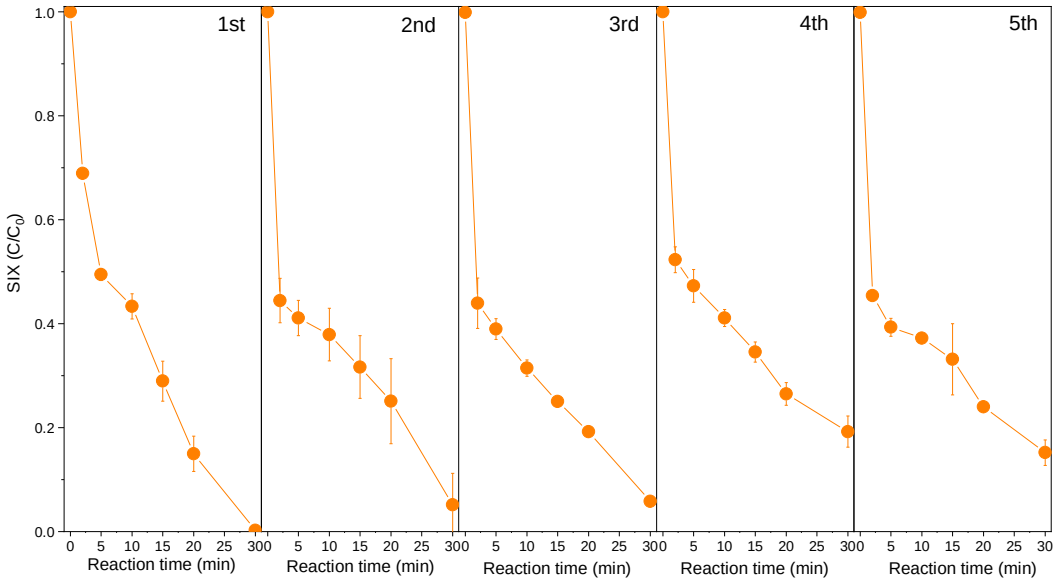


Figure S4. Degradation of SIX by chalcopyrite-PMS oxidation in consecutive catalytic cycles. Conditions: [SIX] = 5 mg/L, [PMS] = 0.5 mM, [chalcopyrite] = 0.5 g/L, and pH 3.0.

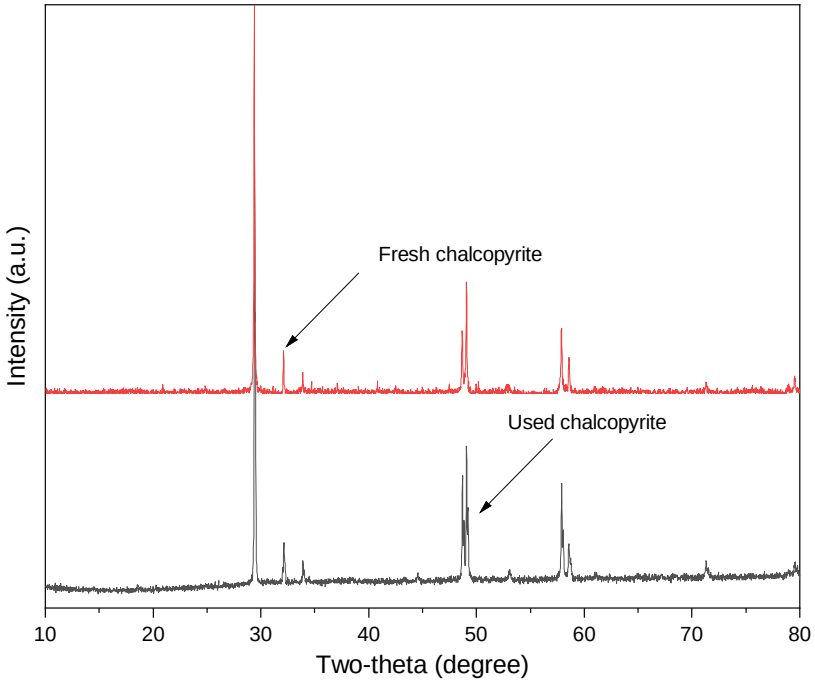


Figure S5. XRD patterns of fresh and used chalcopyrite.

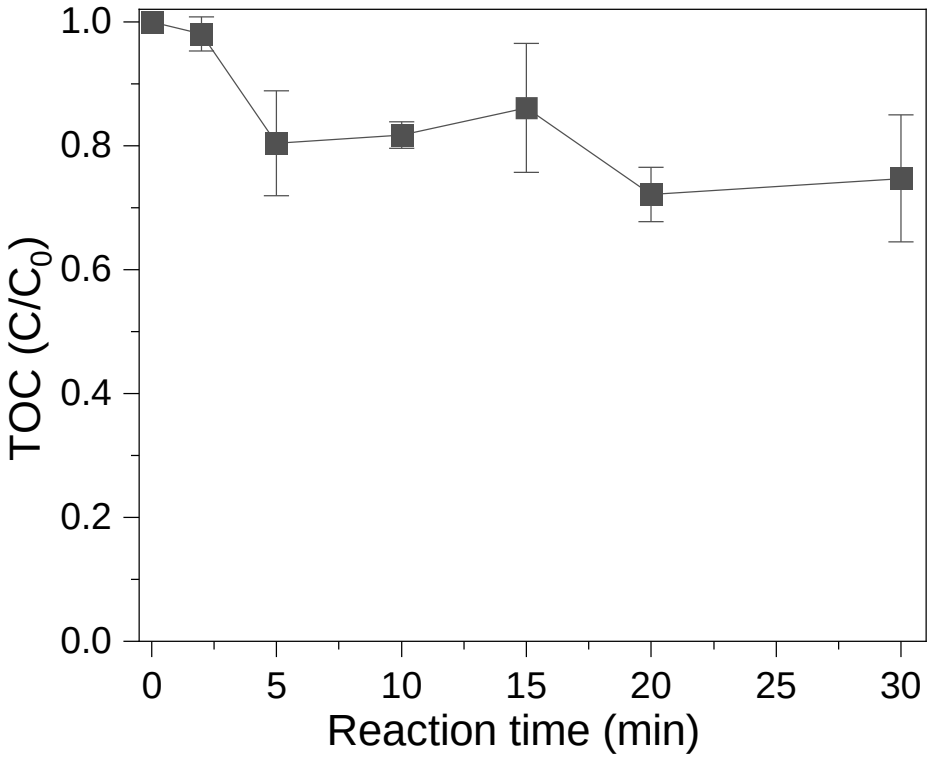


Figure S6. Removal of TOC by chalcopyrite-PMS oxidation. Conditions: [SIX] = 5 mg/L, [PMS] = 0.5 mM, [chalcopyrite] = 1 g/L, and pH 3.0.

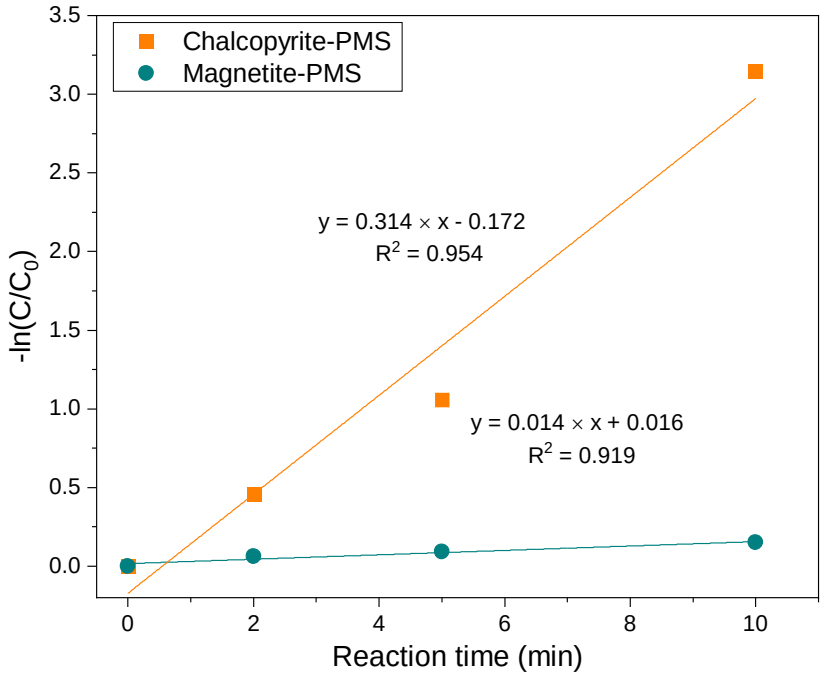


Figure S7. Plot of -ln(C/C$_0$) versus reaction time. The straight line represents linear fitting.

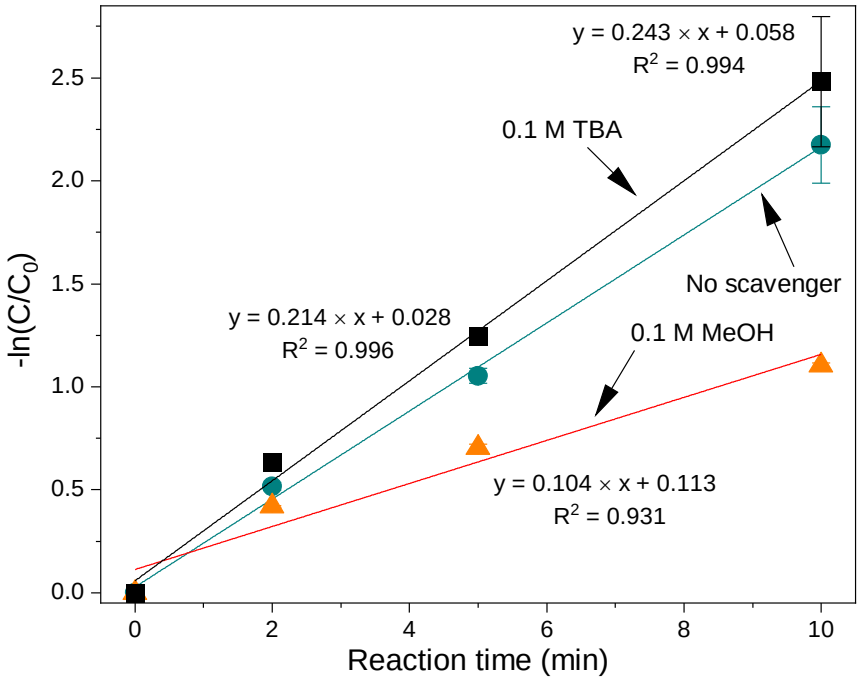


Figure S8. Plot of -ln(C/C$_0$) versus reaction time. The straight line represents linear fitting.

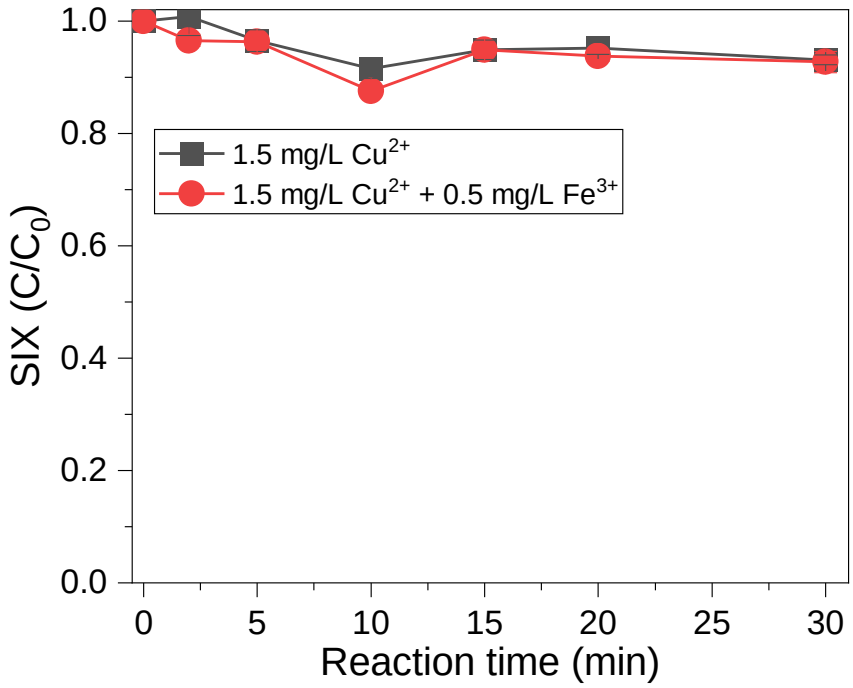


Figure S9. Degradation of SIX by PMS in the presence of Cu^{2+} or both Cu^{2+} and Fe^{3+}. Conditions: [SIX] = 5 mg/L, [PMS] = 0.5 mM, and pH 3.0.

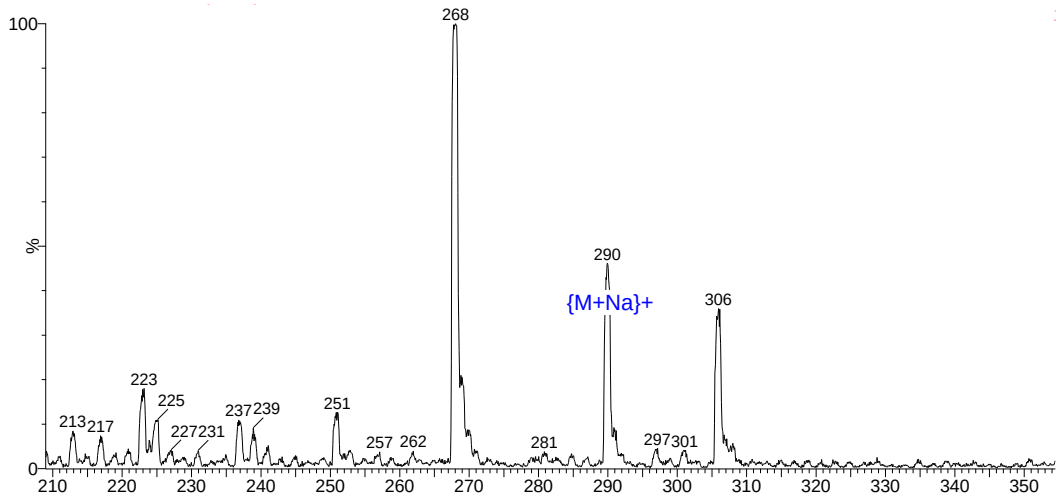


Figure S10. Fragmentation pattern of SIX.

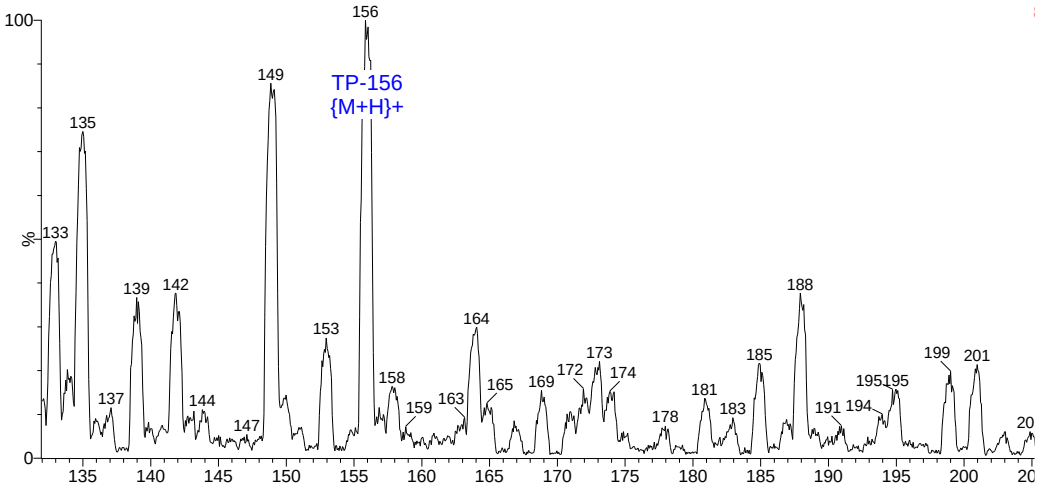


Figure S11. Fragmentation pattern of TP1.

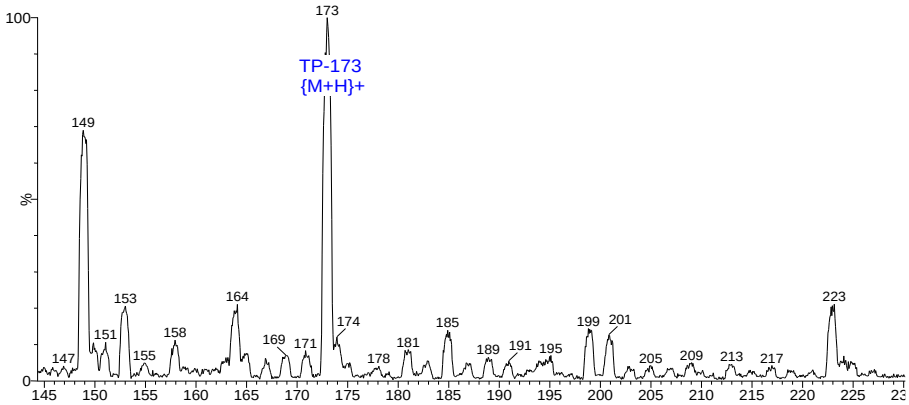


Figure S12. Fragmentation pattern of TP2.

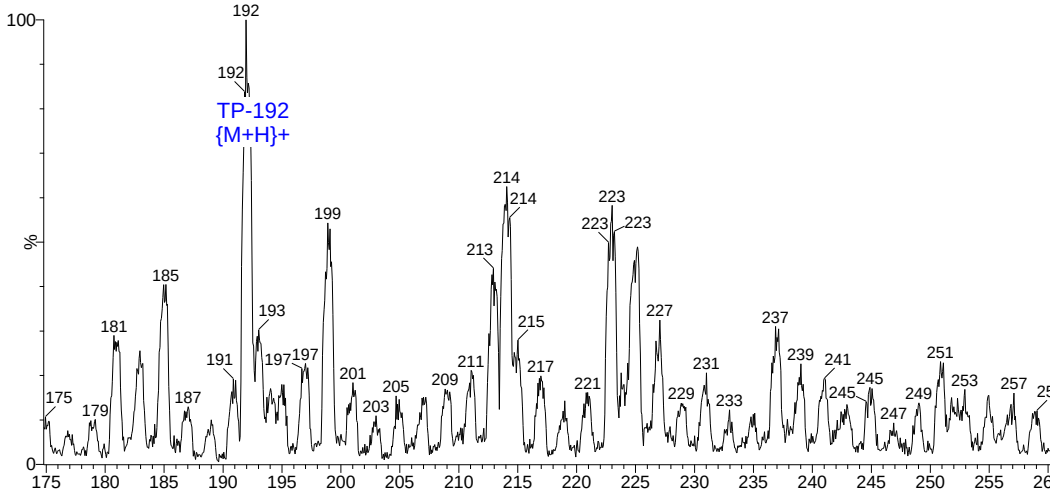


Figure S13. Fragmentation pattern of TP3.

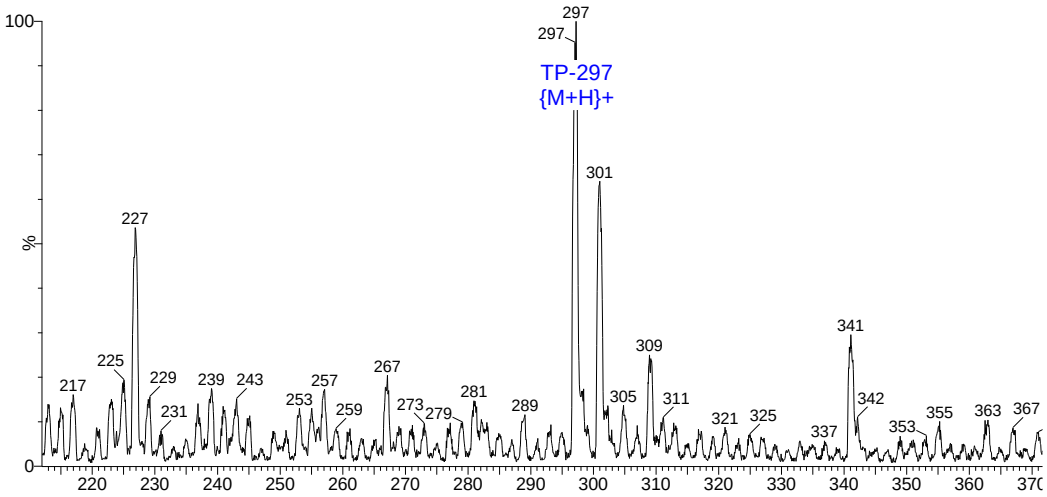


Figure S14. Fragmentation pattern of TP4.

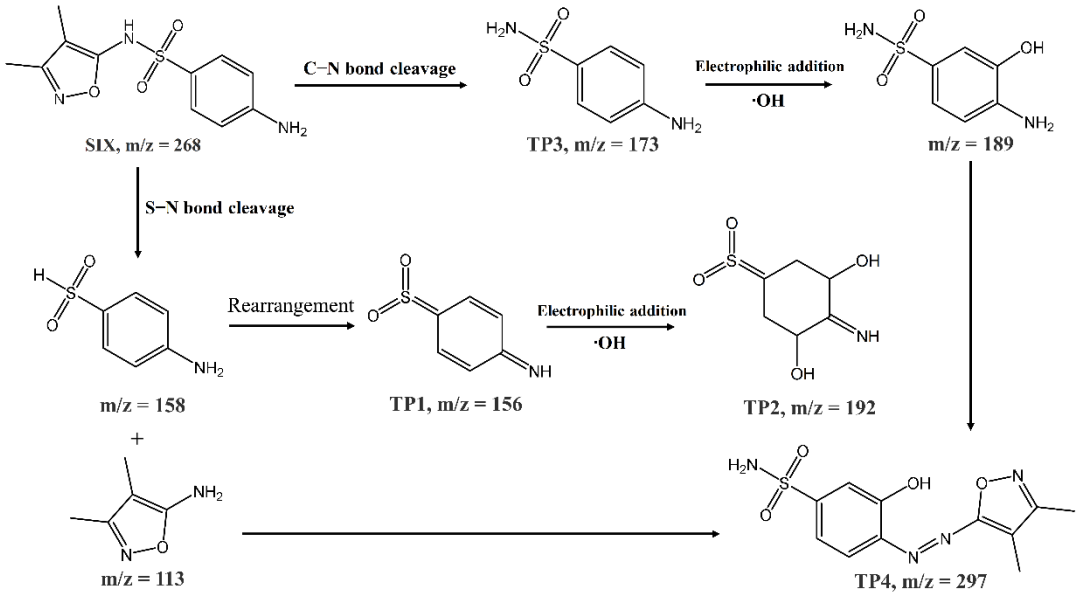


Figure S15. Proposed pathways for the degradation of SIX in chalcopyrite-PMS oxidation.