

Supplementary Information

for

Persulfate activation by nano zero-valent iron for the degradation of metoprolol in water: influencing factors, degradation pathways and toxicity analysis

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Table S1. The major qualities of WWTP effluent.

Sample	pH	TOC (mg/L)	Cl ⁻ (mg/L)	SO ₄ ²⁻ (mg/L)	NO ₃ ⁻ (mg/L)
WWTP effluent	7.02	8.9	57	32	7.1

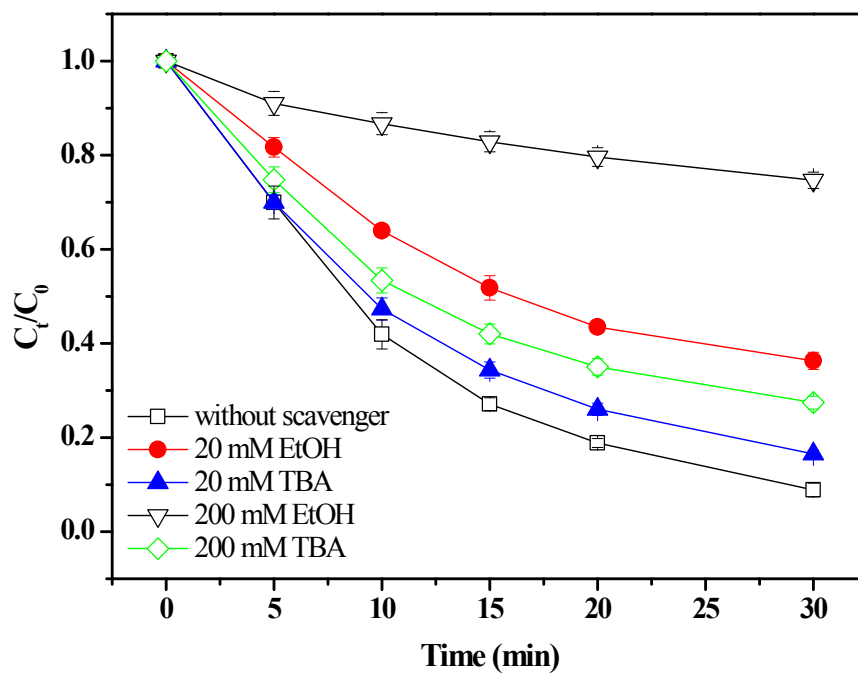


Fig. S1. Effect of EtOH and TBA on MTP degradation in the nZVI/PS system.

Conditions: $[MTP]_0 = 0.05$ mM, $[PS]_0 = 2$ mM, $[nZVI]_0 = 0.33$ g/L, no pH adjustment.

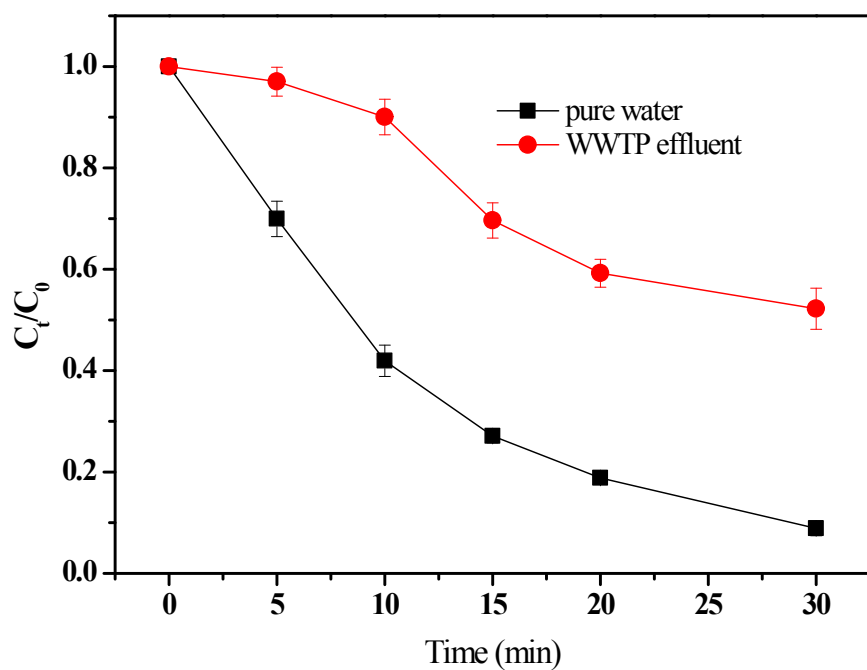
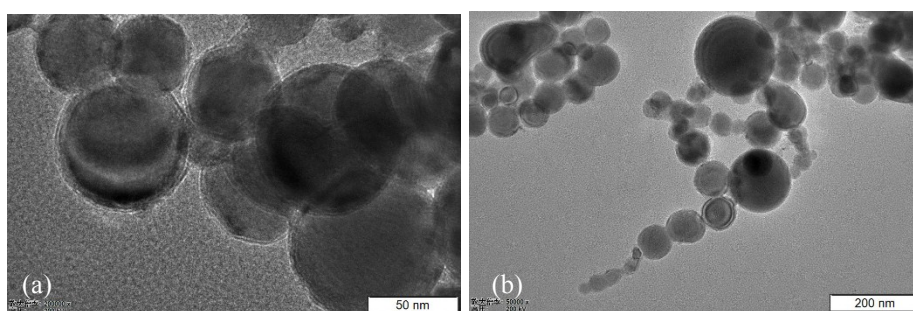


Fig. S2. Degradation of MTP by the nZVI/PS in WWTP effluent.

Conditions: $[MTP]_0 = 0.05$ mM, $[PS]_0 = 2$ mM, $[nZVI]_0 = 0.33$ g/L, no pH adjustment.



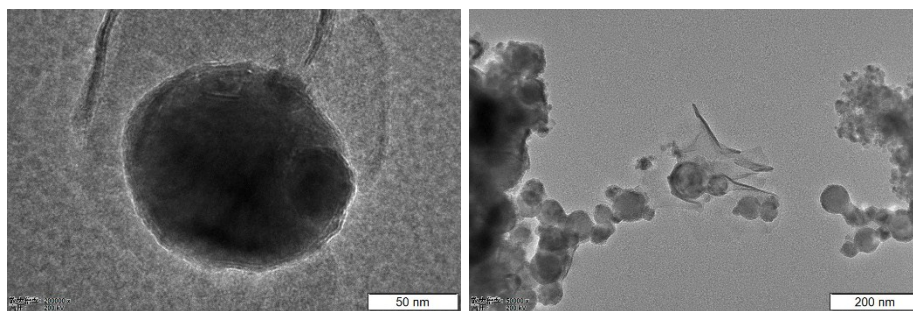


Fig. S3. TEM images of nZVI before (a-b) and after (c-d) reaction.

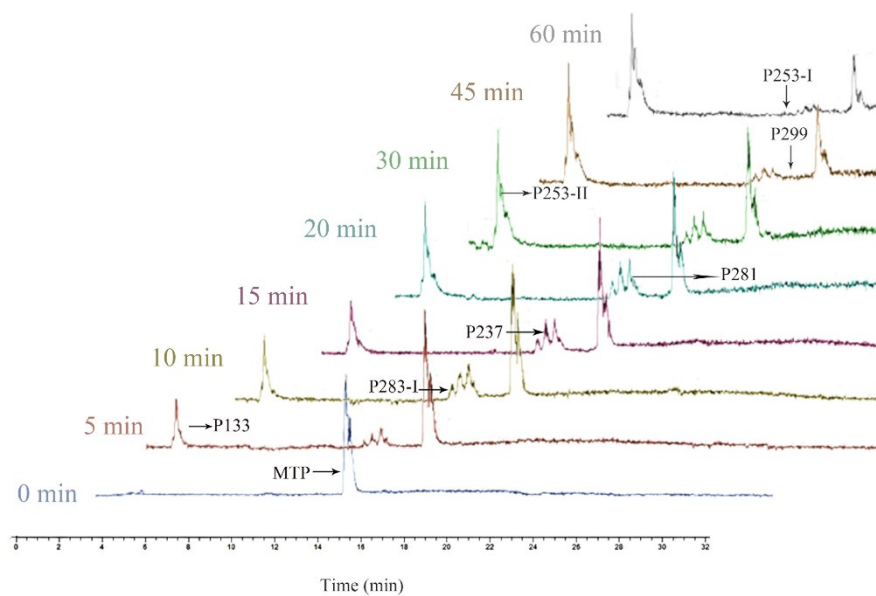
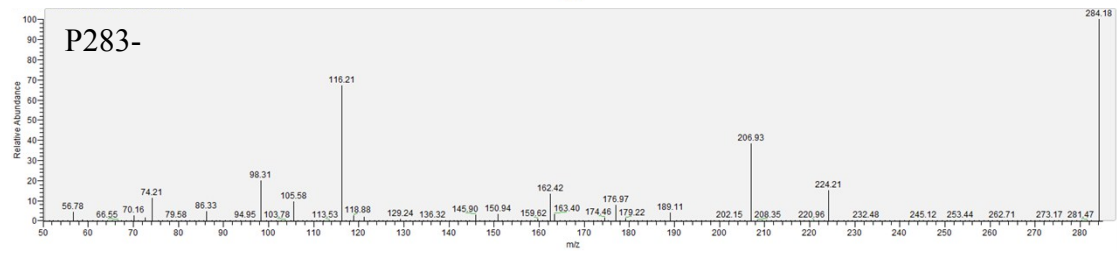
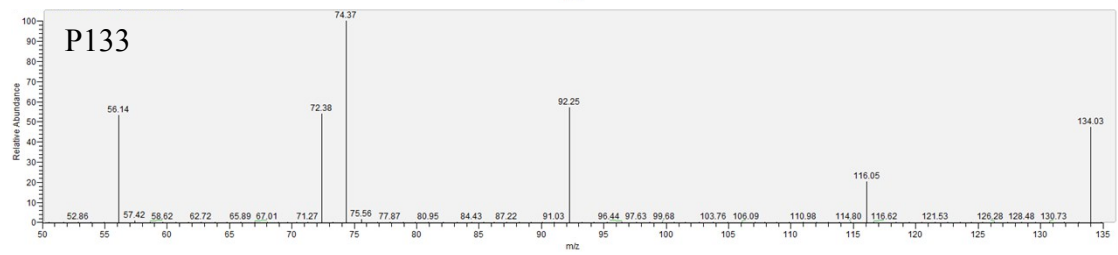
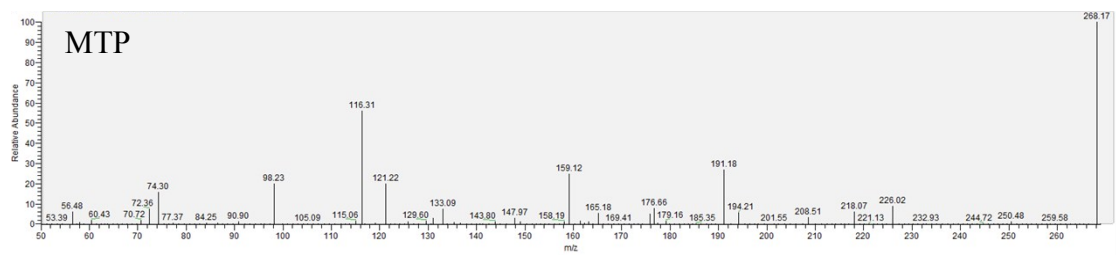


Fig. S4 Total ion current (TIC) chromatograms obtained under different reaction times.



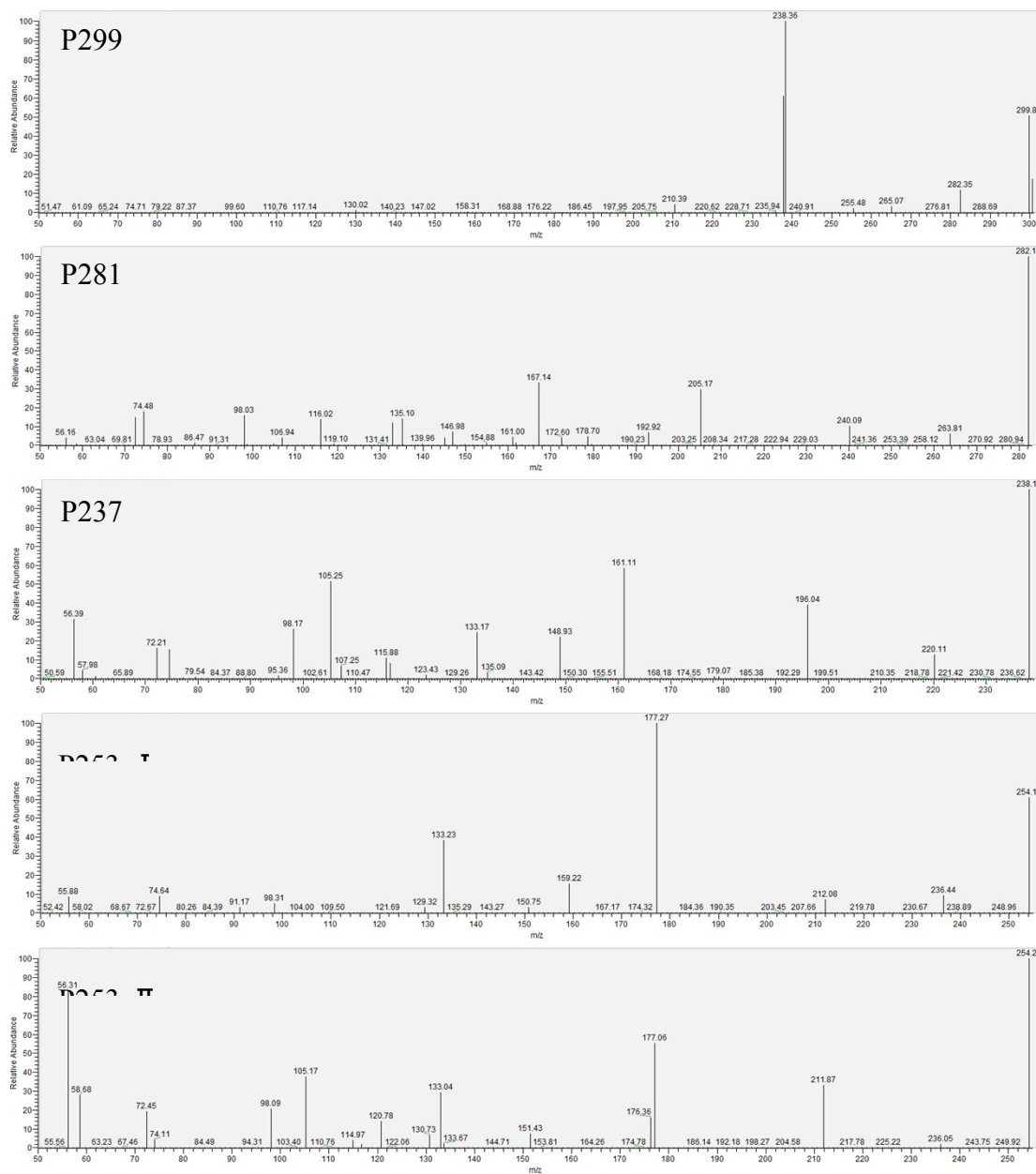
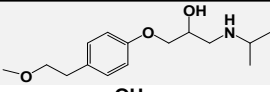
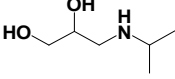
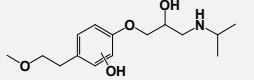
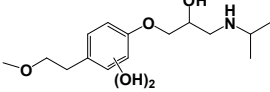
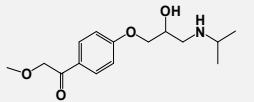
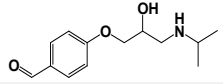
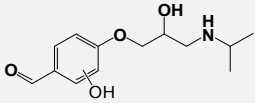
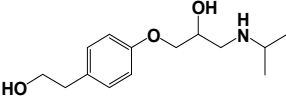


Fig. S5. MS/MS information for MTP and its intermediate products during the reaction.

Table S2. Intermediate products identified for MTP degradation.

Compounds	Retention time (min)	m/z	MS/MS	Structure
MTP	14.74	268	56,74,98,116,133,159,191,226	
P133	2.02	134	56,74,92,116	
P283- I	11.56	284	56,74,98,116,177,207,224	
P299	12.44	300	238,282	
P281	12.39	282	56,74,98,116,167,205,240,263	

P237	11.97	238	56,72,98,105,133,161,196,220	
P253- I	10.91	254-1	56,72,98, 116,133,159,,177,212,236	
P253- II	1.85	254-2	56,72,98,105,121,133,151,177, 212	

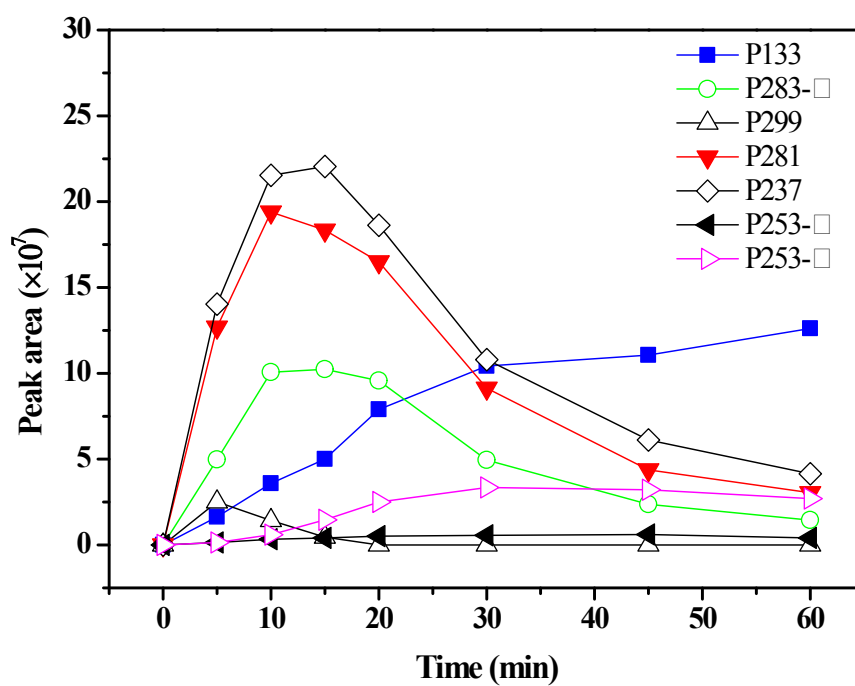


Fig. S6. The time evolution of the peak areas of the identified products.

Conditions: $[\text{MTP}]_0 = 0.05 \text{ mM}$, $[\text{PS}]_0 = 2 \text{ mM}$, $[\text{nZVI}]_0 = 0.33 \text{ g/L}$, no pH adjustment.