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Supplementary material: Optimization parameters, kinetics and mechanism of naproxen removal by catalytic wet peroxide oxidation with a hybrid iron-based magnetic catalyst

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Table S1. Comparison of iron-based catalytic systems for the removal of NAP in liquid phase.

Treatment process	Experimental conditions	Initial concentration, mg/L	Removal efficiency, %	Reference
Homogeneous Fenton	$[Fe^{2+}]$ = 4.83mg/L; $[H_2O_2]_0$ = 9.98 mM	20.0	100.0	[1]
Fenton-like oxidation	pH = 3; 28-33 °C MGO = 1 g/L; 25 °C; pH = 3; $[H_2O_2]$ = 5 mM	2.3	100.0	[2]
Fenton-like oxidation	citric acid (CA) $[Fe^{2+}]_0$ = $[CA]_0$ = 75 μM; ion ; 25 °C; $[S_2O_8{}^{2-}]_0$ = 750 μM	17.2	99.9	[3]
Homogeneous sonocatalytic process (US/Fenton/TiO_2)	Fe^{2+}:H_2O_2=20/4 1000 kHz; pH = 3; 20 °C	0.23	96.0	[4]
Heterogeneous sonocatalytic process	60 kHz; pH = 4.5; [ZnO/MMT]=11 g/L	10	82.0	[5]
Magnetite supported on multiwalled carbon nanotubes	Cat = 1g/L; 70 °C, $[H_2O_2]_0$ = 1.5 mM; pH 5	10	82.0	This work

Table S2. NAP degradation products detected by (-)-ESI-LC-MS analysis.

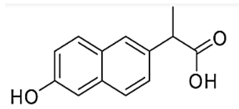
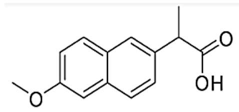
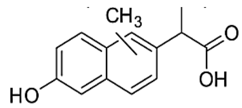
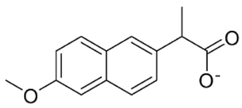
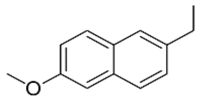
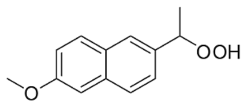
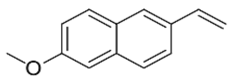
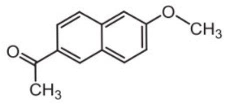
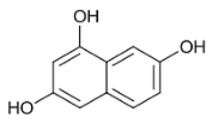
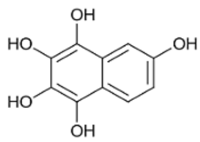
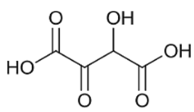
Compound	Molecular weight	$[M+H]^+$, m/z	Reaction pathway	Chemical structure
C1	216	217	+[HO] -[CH_3O]	
C2	229	230	*	
C3	230	231	+[HO] -[CH_3O] +[CH_3]	
C4	228	229	-[H]	
C5	186	187	-[COO]	
A	218	219	+2[HO] -[H] -[COOH]	
C6	184	185	+[HO] -[H_2O] -[COOH]	
C7	200	201	+[HO] -2[H] -[COOH]	
C8	176	177	+3[HO] -[CH_3O] -[COOH] -[C_3H_5]	
C9	208	209	+5[HO] -[CH_3O] -[COOH] -[C_3H_5]	
B	148	149	+10[HO] -[CH_3O] -7[COOH] -[C_3H_5]	

Table S3. Representative analysis of the three real-aqueous matrices.

	Hospital water	Surface water	WWTP effluent
pH	8.6	6.1	7.4
Conductivity (mS/cm^2)	1.17	0.1641	0.557
COD (mg/L)	365	16	18
TOC (mg/L)	110	6.8	9.8
Suspended solids (mg/L)	138	140	80
Aromaticity (a.u)	0.50	0.16	0.12
Phenolic compounds (mg/L)	8.9	$9.8 \cdot 10^{-4}$	0.002
TN (mg/L)	94	0.98	0.87
NH^{4+} (mg/L)	75	2.43	0.8
NO^{3-} (mg/L)	0.64	1.84	0.0201

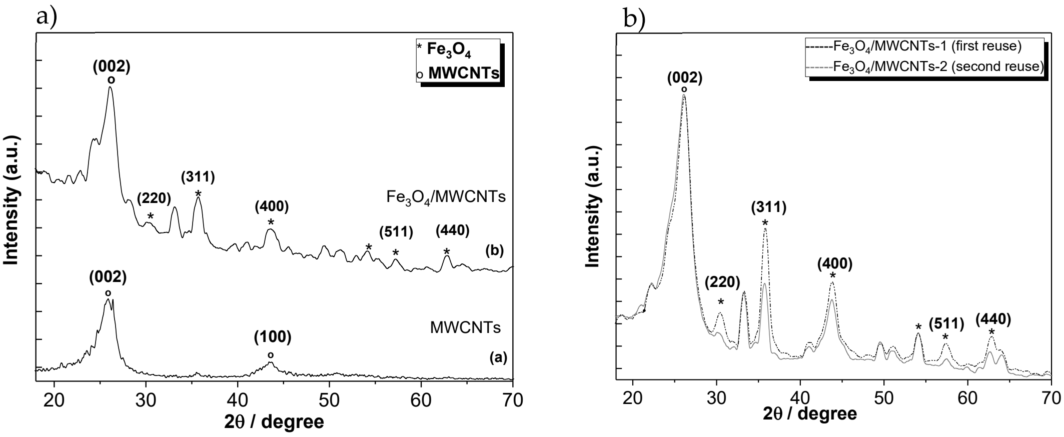


Figure S1. XRD patterns of (**a**) magnetite (Fe_3O_4) and catalytic support; (**b**) Fe_3O_4/MWCNTs-1 and Fe_3O_4/MWCNTs-2 catalysts.

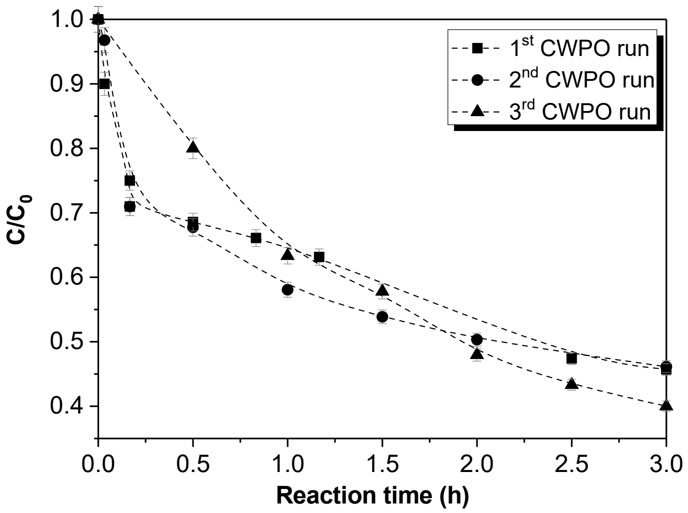


Figure S2. Evolution of H_2O_2 efficiency along the three CWPO runs.

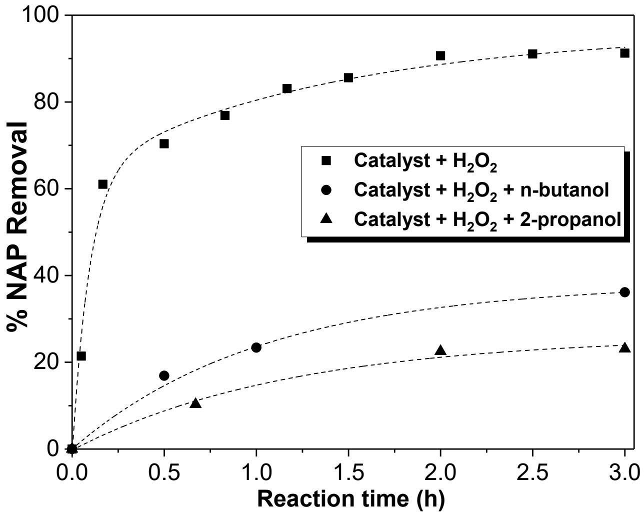
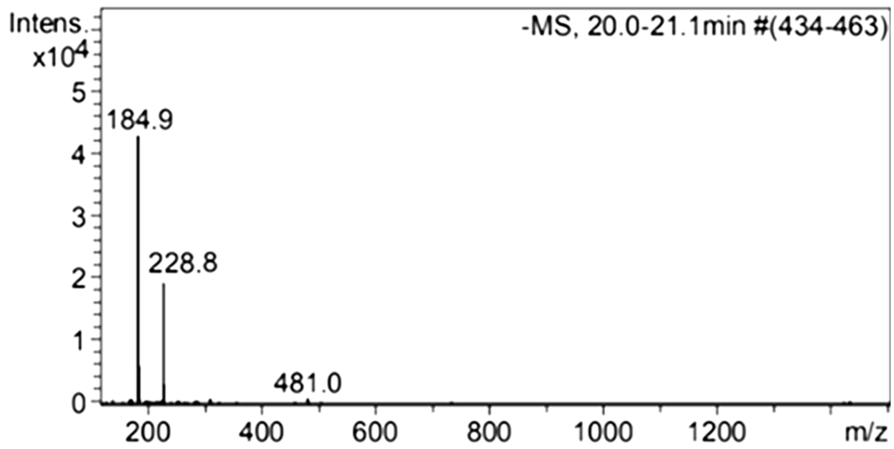
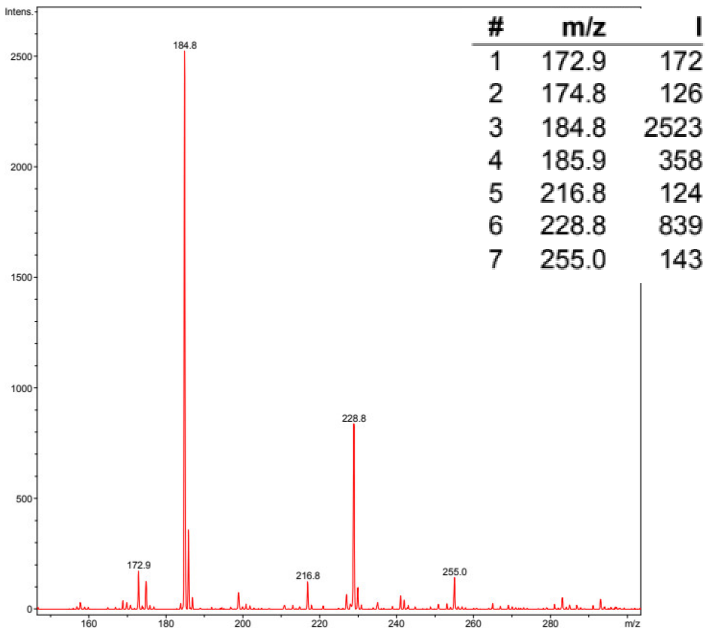


Figure S3. Quenching tests of hydroxylradicals in the CWPO reaction.



#	m/z	I
1	128.9	106
2	140.8	398
3	168.8	112
4	169.9	436
5	170.9	112
6	172.8	519
7	174.9	265
8	184.9	42709
9	185.9	5924
10	186.9	558
11	198.8	272
12	200.9	124
13	208.9	116
14	212.9	108
15	216.9	243
16	228.2	383
17	228.8	19173
18	229.8	2875
19	230.9	320
20	255.0	205
21	286.8	211
22	310.9	471
23	311.8	110
24	481.0	694
25	482.0	176
26	733.1	109

Figure S4. Chromatogram of NAP treated byCWPO reaction.



#	m/z	I
1	172.9	172
2	174.8	126
3	184.8	2523
4	185.9	358
5	216.8	124
6	228.8	839
7	255.0	143

Figure S5. Chromatogram of NAP standard.

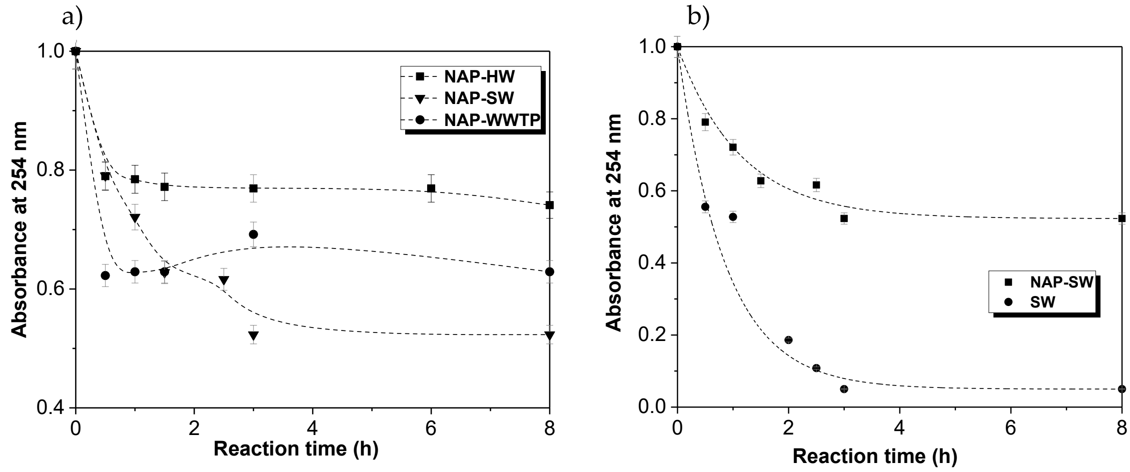


Figure S6. Evolution of the aromaticity content (**a**) for the three tested real-aqueous matrices spiked with NAP; (**b**) for SW sample and SW sample spiked with NAP.

References

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