

Supporting information:

Degradation of Paracetamol by an UV/Chlorine Advanced Oxidation Process: Influencing Factors, Factorial Design, and Intermediates Identification

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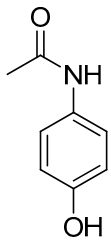
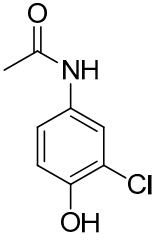
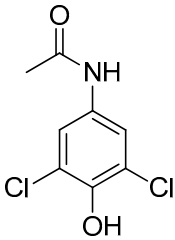
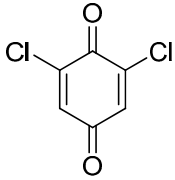
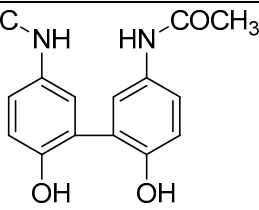
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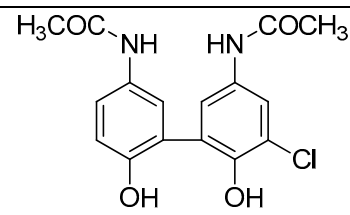
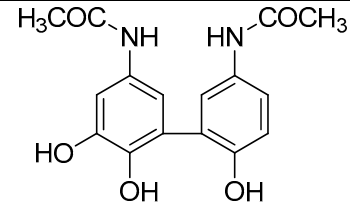
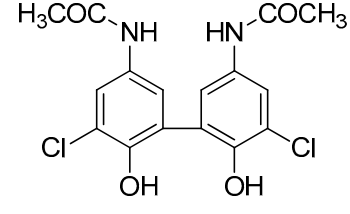
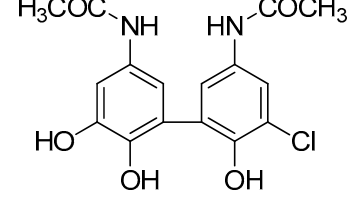
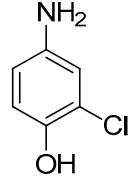
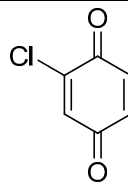
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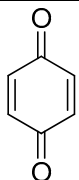
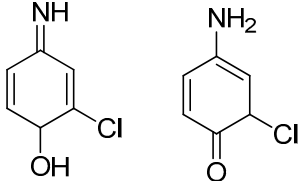
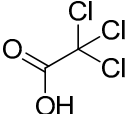
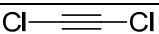
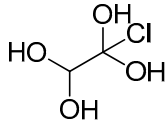
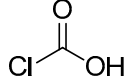
Table S1. The RSM experiment design matrix and experimental results

Exp	Run order	Coded variable				Independent variables				Removal efficiency (%)	
		X ₁	X ₂	X ₃	X ₄	UV	pH	NaOCl	DOM	Experiment	Model
1	1	-1	-1	-1	-1	3.41	4	50	2	19.4	21.2
2	18	1	-1	-1	-1	10.23	4	50	2	25.7	28.1
3	22	-1	1	-1	-1	3.41	9	50	2	18.9	21.2
4	19	1	1	-1	-1	10.23	9	50	2	24.6	28.1
5	6	-1	-1	1	-1	3.41	4	150	2	50.8	50.0
6	9	1	-1	1	-1	10.23	4	150	2	55.9	56.9
7	7	-1	1	1	-1	3.41	9	150	2	49.6	50.0
8	14	1	1	1	-1	10.23	9	150	2	53.6	56.9
9	4	-1	-1	-1	1	3.41	4	50	5	8.6	7.2
10	17	1	-1	-1	1	10.23	4	50	5	15.5	14.0
11	12	-1	1	-1	1	3.41	9	50	5	7.8	7.2
12	20	1	1	-1	1	10.23	9	50	5	14.2	14.0
13	13	-1	-1	1	1	3.41	4	150	5	42.5	36.0
14	28	1	-1	1	1	10.23	4	150	5	46.8	42.8
15	8	-1	1	1	1	3.41	9	150	5	41.6	36.0
16	16	1	1	1	1	10.23	9	150	5	45.2	42.8
17	26	-2	0	0	0	0.00	6.5	100	3.5	38.5	40.5
18	11	2	0	0	0	13.64	6.5	100	3.5	58.7	54.3
19	5	0	-2	0	0	6.82	1.5	100	3.5	6.5	7.5
20	29	0	2	0	0	6.82	11.5	100	3.5	6.3	7.5
21	21	0	0	-2	0	6.82	6.5	0	3.5	1.1	18.6
22	23	0	0	2	0	6.82	6.5	200	3.5	48.2	76.2
23	3	0	0	0	-2	6.82	6.5	100	0.5	70.5	39.7
24	15	0	0	0	2	6.82	6.5	100	6.5	24.6	11.7
25	2	0	0	0	0	6.82	6.5	100	3.5	50.2	47.4
26	10	0	0	0	0	6.82	6.5	100	3.5	45.5	47.4
27	27	0	0	0	0	6.82	6.5	100	3.5	46.7	47.4
28	31	0	0	0	0	6.82	6.5	100	3.5	42.5	47.4
29	24	0	0	0	0	6.82	6.5	100	3.5	41.2	47.4
30	30	0	0	0	0	6.82	6.5	100	3.5	52.3	47.4
31	25	0	0	0	0	6.82	6.5	100	3.5	46.5	47.4

Table S2. Accurate mass measurement of product ions of PRC and its transformed products identified by LC/MS/MS

Compound symbol	m/z, [M+/-X]	RT	Proposed formula
1	152.06334, [M+1]	6.10	 <p>Chemical Formula: C₈H₉NO₂ Exact Mass: 151.06334</p>
2	186.02430, [M+1]	7.56	 <p>Chemical Formula: C₈H₈ClNO₂ Exact Mass: 185.02430</p>
3	219.00610, [M+1]	8.76	 <p>Chemical Formula: C₈H₇Cl₂NO₂ Exact Mass: 218.00610</p>
4	174.94330, [M-1]	5.59	 <p>Chemical Formula: C₆H₂Cl₂O₂ Exact Mass: 175.94330</p>
5	301.11105, [M+1]	7.01	 <p>Chemical Formula: C₁₆H₁₆N₂O₄ Exact Mass: 300.11105</p>

6	335.07210, [M+1]	7.98	 <p>Chemical Formula: C₁₆H₁₅ClN₂O₄ Exact Mass: 334.07210</p>
7	317.10599, [M+1]	8.65	 <p>Chemical Formula: C₁₆H₁₆N₂O₅ Exact Mass: 316.10599</p>
8	369.03312, [M+1]	8.66	 <p>Chemical Formula: C₁₆H₁₄Cl₂N₂O₄ Exact Mass: 368.03312</p>
9	351.06700, [M+1]	14.72	 <p>Chemical Formula: C₁₆H₁₅ClN₂O₅ Exact Mass: 350.06700</p>
10	144.01400, [M+1]	8.67	 <p>Chemical Formula: C₆H₆ClNO Exact Mass: 143.01400</p>
11	140.98219, [M-1]	9.11	 <p>Chemical Formula: C₆H₃ClO₂ Exact Mass: 141.98219</p>

12	107.02114, [M-1]	6.00	 <p>Chemical Formula: C₆H₄O₂ Exact Mass: 108.02114</p>
13	144.01400, [M+1]	10.1 and 10.5	 <p>Chemical Formula: C₆H₆ClNO Exact Mass: 143.01400</p>
14	160.90427; [M-1]	2.6	 <p>Chemical Formula: C₂HCl₃O₂ Exact Mass: 161.90427</p>
15	140,95883; [M-1]	2,52	<p>Chemical Formula: C₃H₄Cl₂O₂ Exact Mass: 141.95883</p>
16	92,93779; [M-1]	2,50	 <p>Chemical Formula: C₂Cl₂ Exact Mass: 93.93779</p>
17	138,96395; [M+1]	2,42	<p>Chemical Formula: C₄H₄Cl₂O Exact Mass: 137.96395</p>
18	128,98769; [M+1]	2,60	 <p>Chemical Formula: C₂H₅ClO₄ Exact Mass: 127.98769</p>
19	80,96654; [M+1]	2,50	 <p>Chemical Formula: CHClO₂ Exact Mass: 79.96654</p>
20	78,98729; [M+1]	2,32	<p>Chemical Formula: C₂H₃ClO Exact Mass: 77.98729</p>

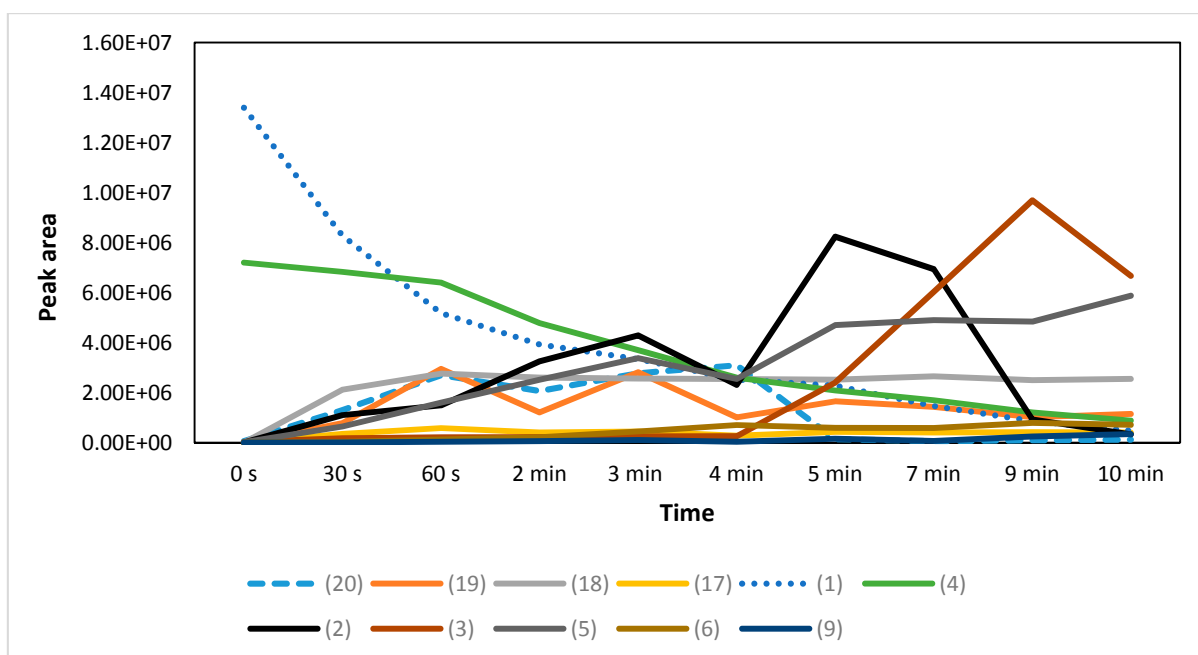
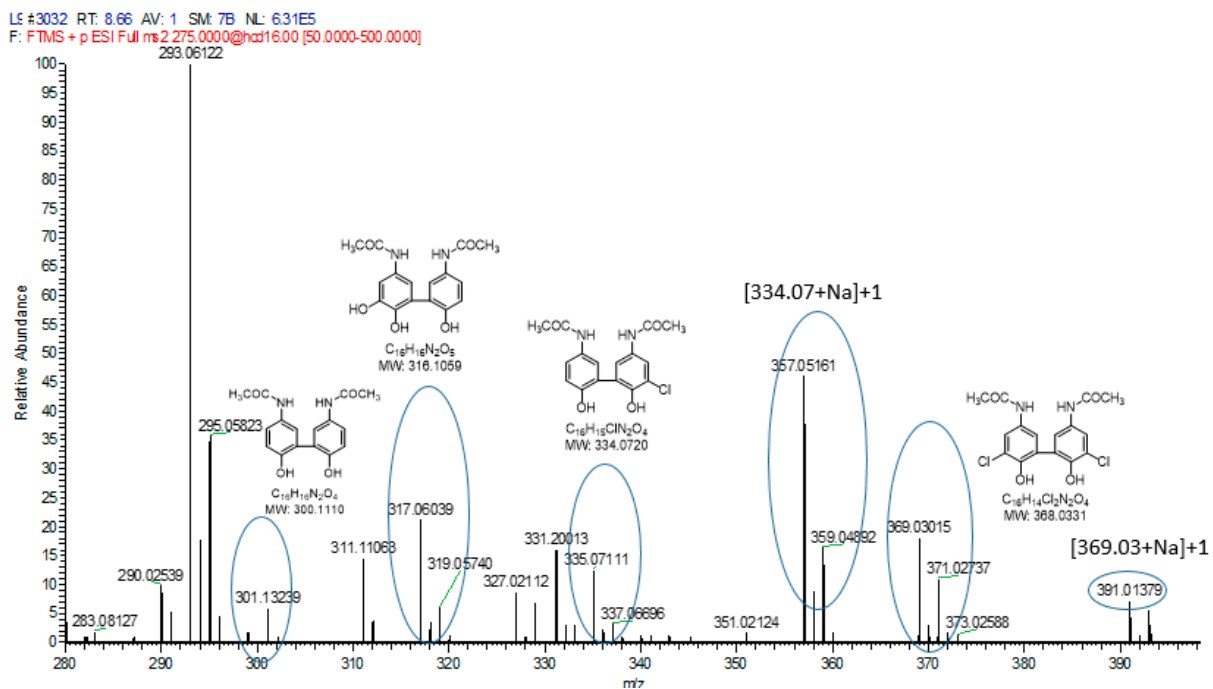
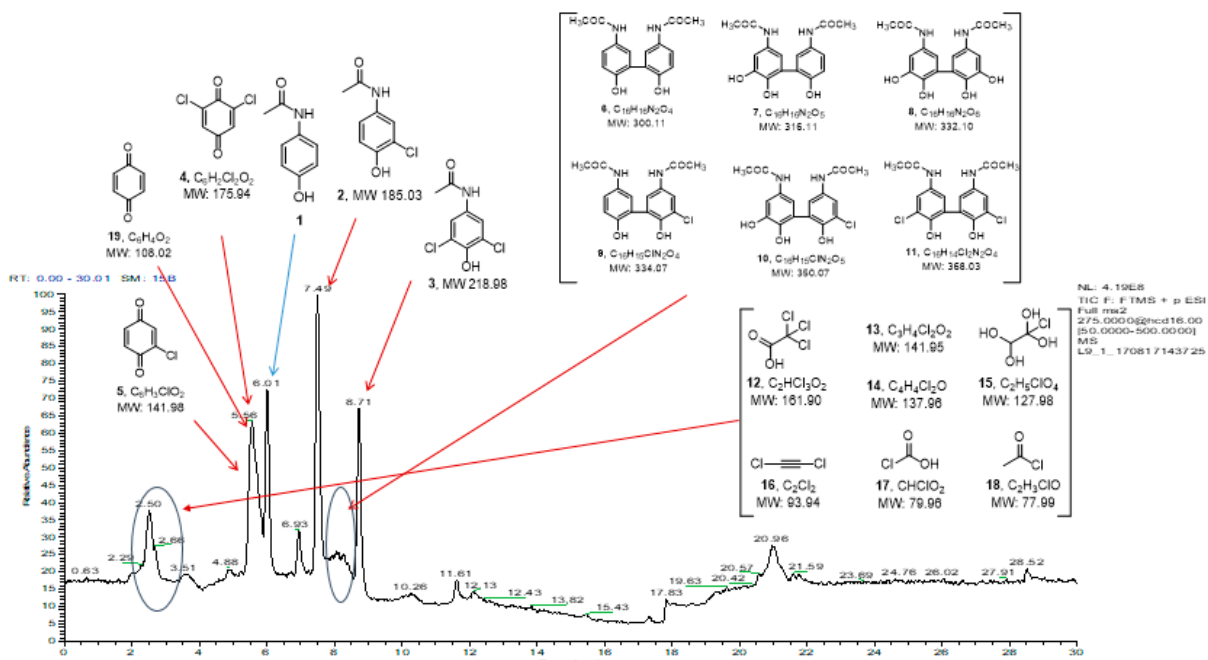


Figure S1. Change of signal peak areas of main transformation products within 10 min



Section S2. Result of liquid chromatography-tandem mass spectrometry (LC-MS/MS) of proposed compound