Supplementary Information

for

Kinetics and mechanistic investigation into the degradation of naproxen by UV/chlorine process

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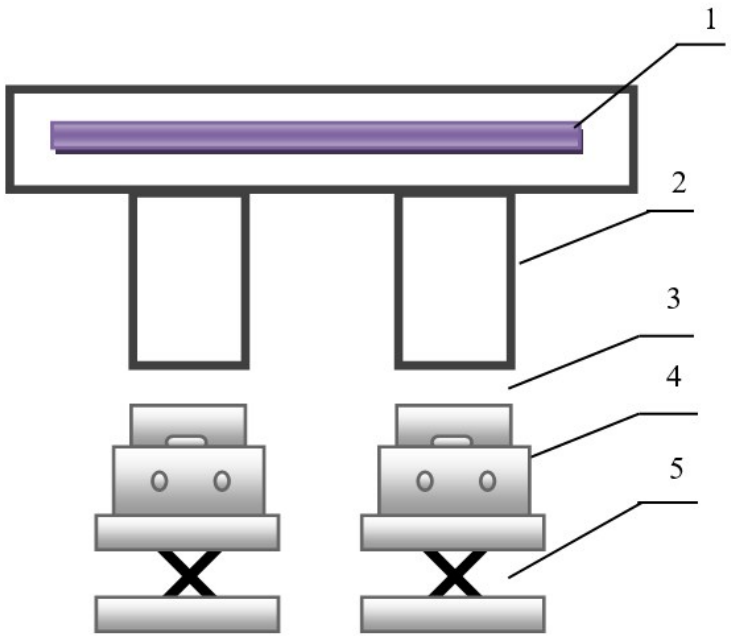


Fig. S1. Schematic description of the reactor

(1. UV lamp; 2. Lampshade; 3. Reaction dish; 4. Magnetic stirrer; 5. Rest pier)

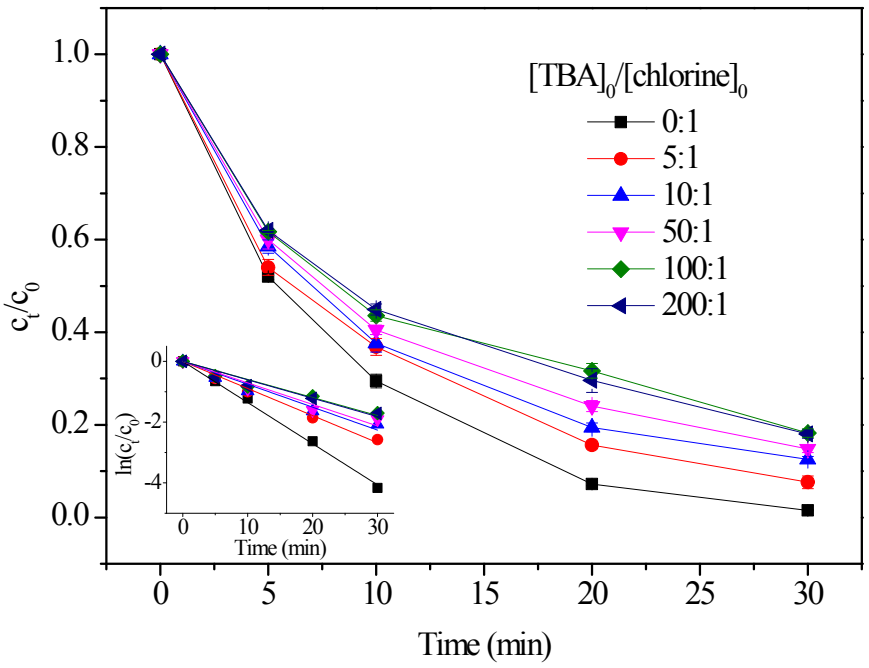
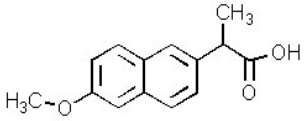
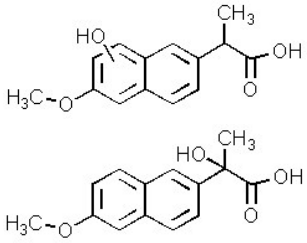
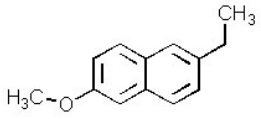
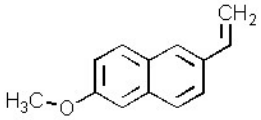
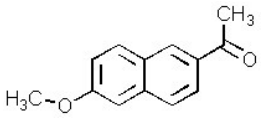
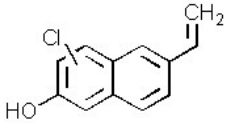
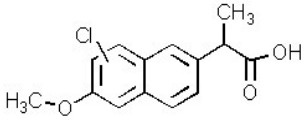
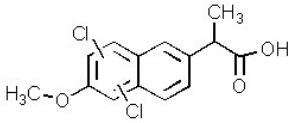
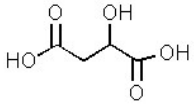
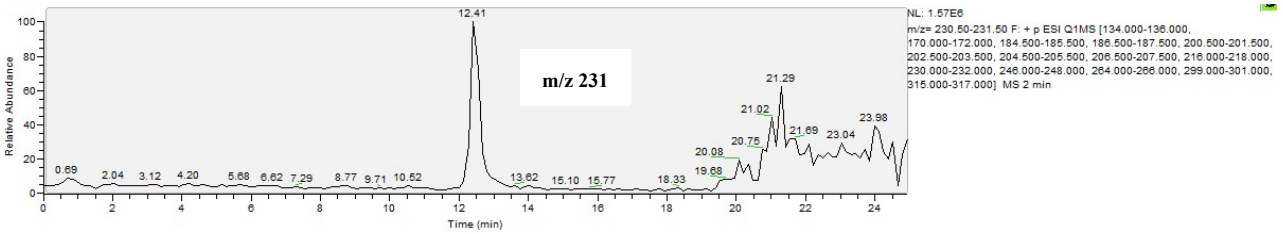


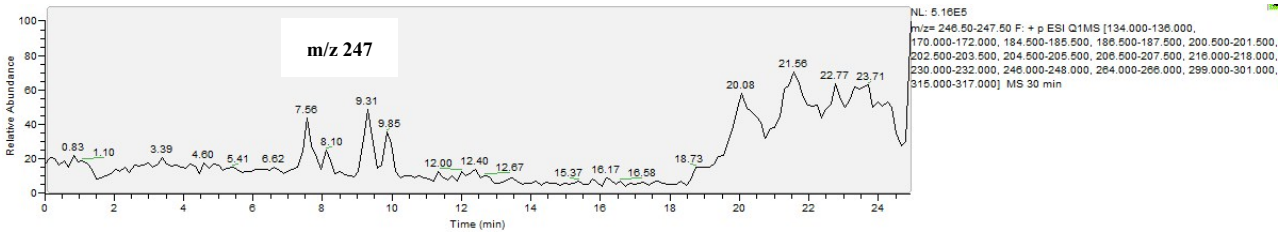
Fig. S2. Effect of different ratios of $[TBA]_0/[NPX]_0$ on NPX degradation by UV/chlorine process

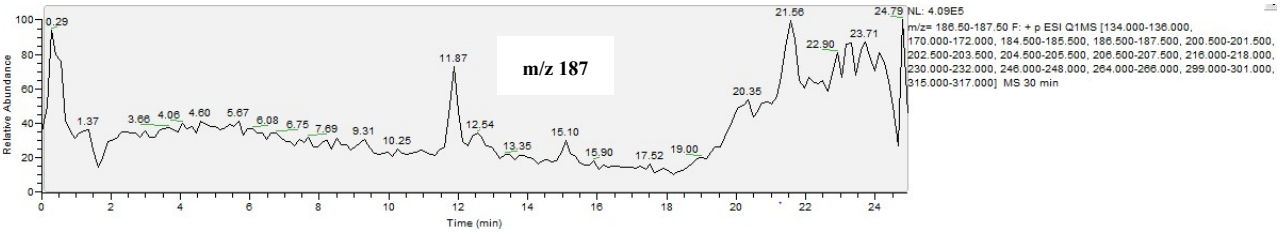
Conditions: $[NPX]_0$ = 25 μM, $[chlorine]_0$ = 250 μM, $[TBA]_0/[chlorine]_0$ = 0~200:1, pH = 7

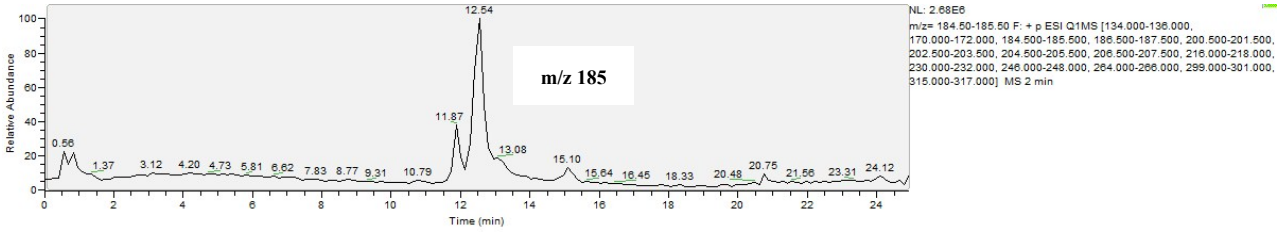
Table S1 Identified NPX intermediate products using LC/MS/MS in UV/chlorine process.

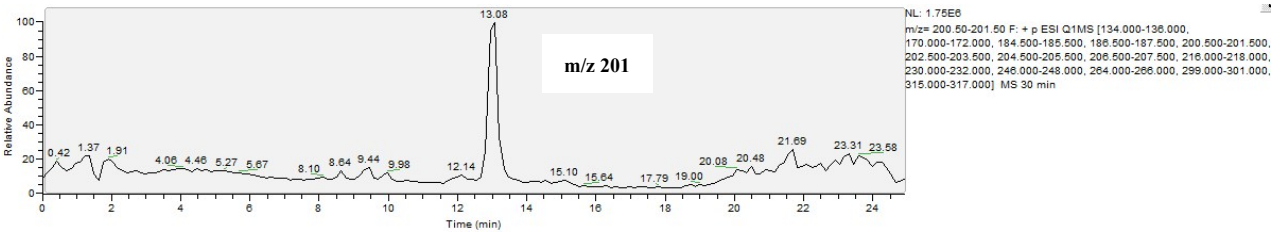
Compound	Retention time (min)	m/z	molecular structure
NPX	12.41	231	
P246	7.56, 9.31	247	
P186	11.87	187	
P184	12.54	185	
P200	13.08	201	
P204	7.56	205	
P264	8.64	265	
P299	16.04	300	
P134	1.50	135	

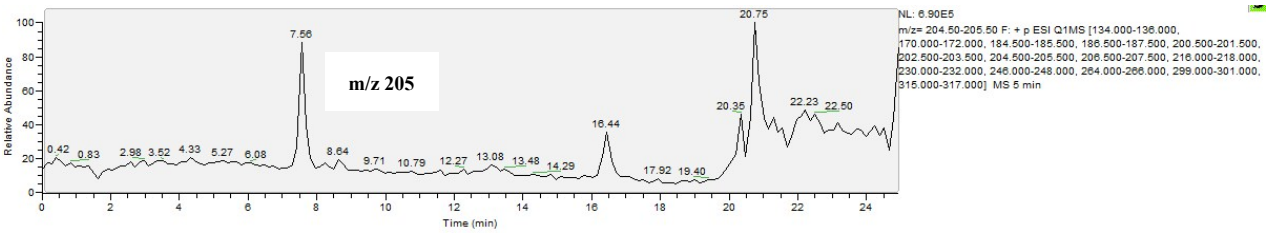

m/z 231
Relative Abundance
Time (min)
NL: 1.57E6
m/z= 230.50-231.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 2 min

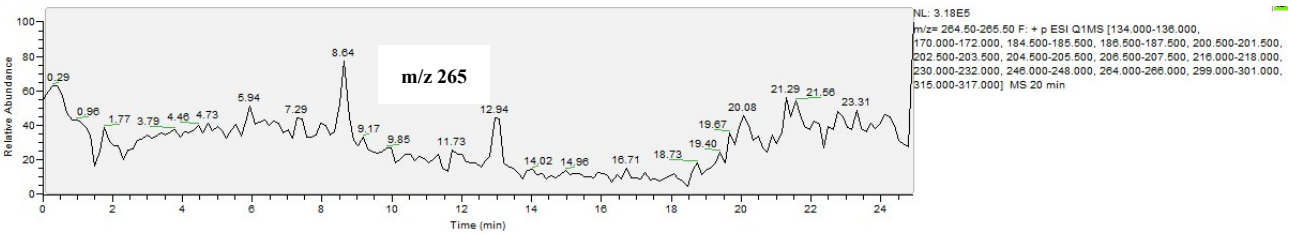

m/z 247
Relative Abundance
Time (min)
NL: 5.16E5
m/z= 246.50-247.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 30 min


m/z 187
Relative Abundance
Time (min)
NL: 4.09E5
m/z= 186.50-187.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 30 min


m/z 185
Relative Abundance
Time (min)
NL: 2.68E6
m/z= 184.50-185.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 2 min


m/z 201
Relative Abundance
Time (min)
NL: 1.75E6
m/z= 200.50-201.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 30 min


m/z 205
Relative Abundance
Time (min)
NL: 6.90E5
m/z= 204.50-205.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 5 min


m/z 265
Relative Abundance
Time (min)
NL: 3.18E5
m/z= 264.50-265.50 F: + p ESI Q1MS [134.000-136.000, 170.000-172.000, 184.500-185.500, 186.500-187.500, 200.500-201.500, 202.500-203.500, 204.500-205.500, 206.500-207.500, 216.000-218.000, 230.000-232.000, 246.000-248.000, 264.000-266.000, 299.000-301.000, 315.000-317.000] MS 20 min

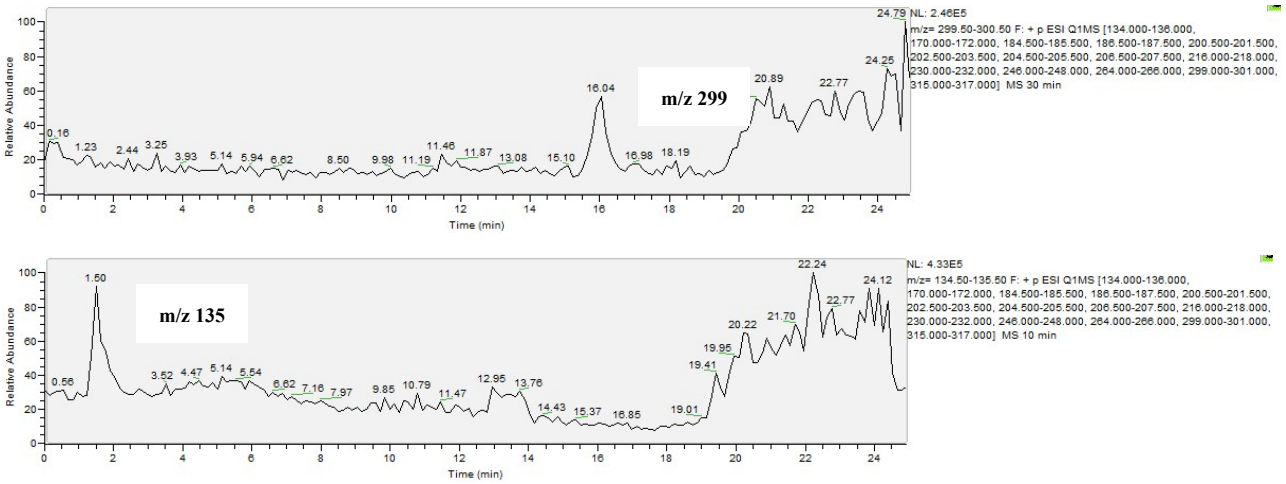
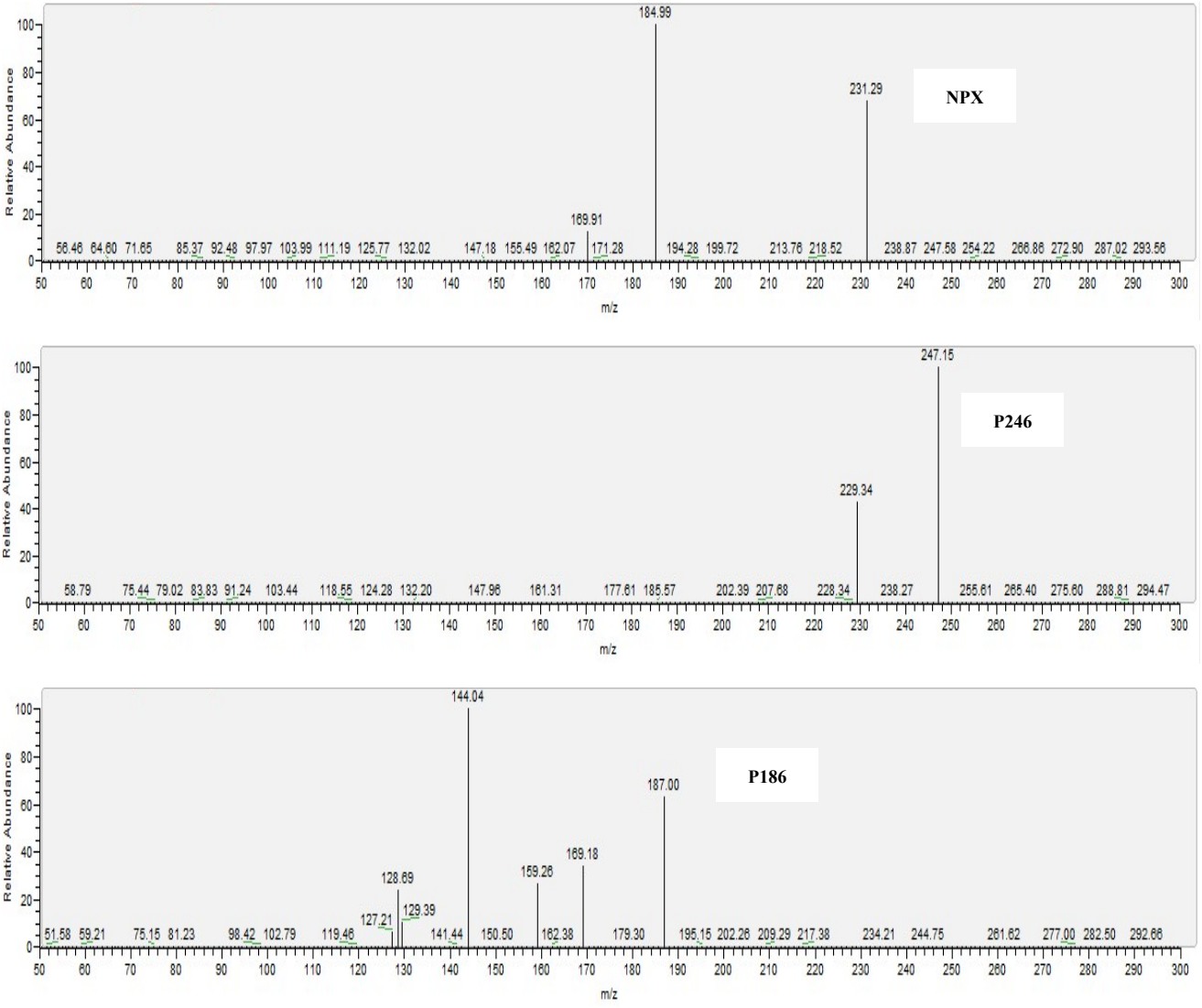
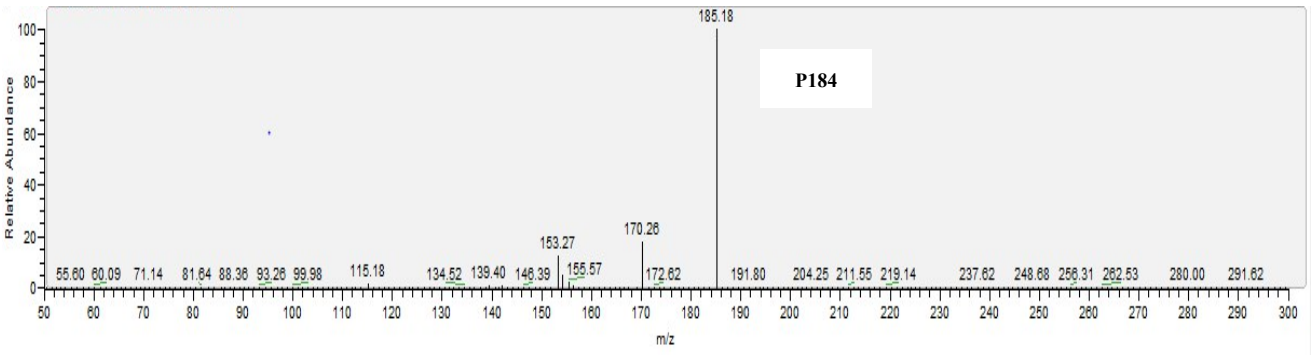
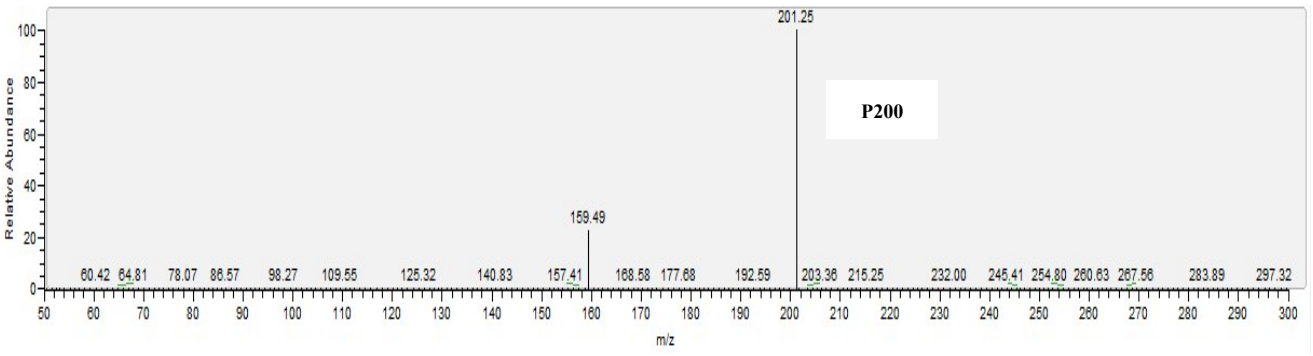
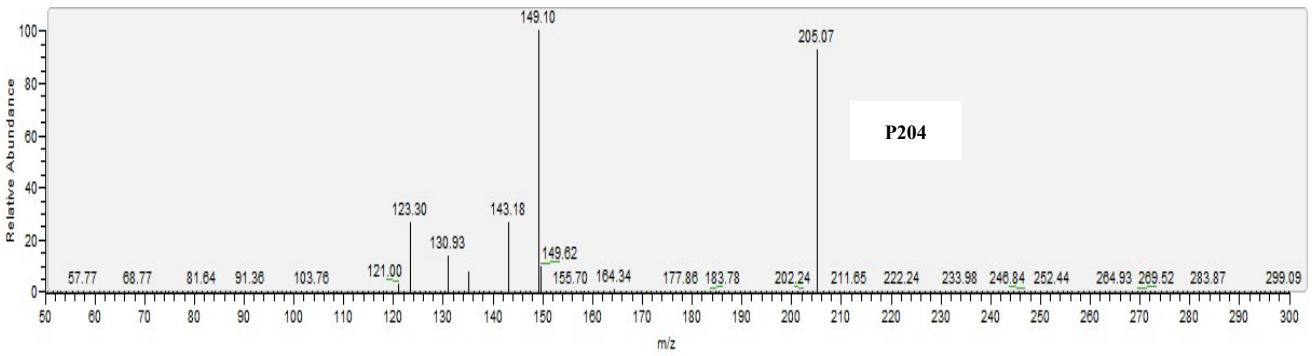


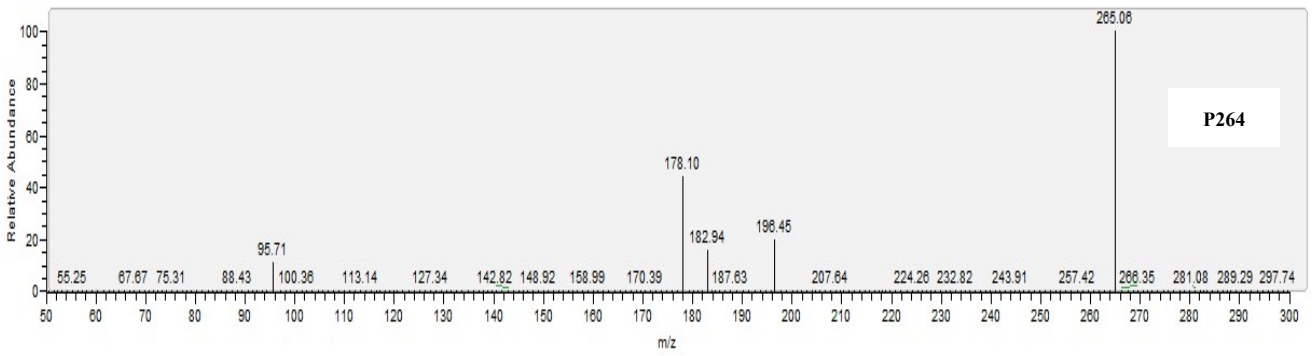
Fig. S3. The LC/MS scan of byproducts of NPX formed during UV/chlorine process by extracting the m/z of ions.

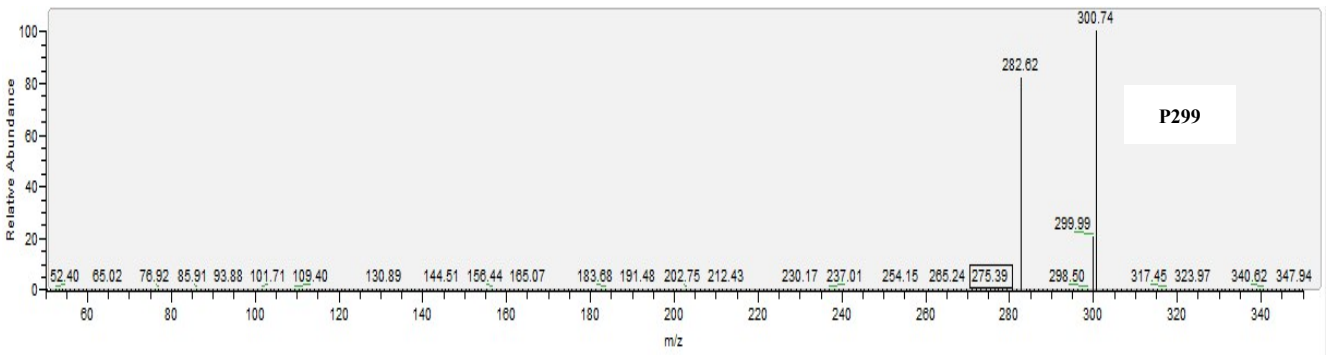



P184
185.18
170.26
163.27
Relative Abundance
m/z


P200
201.25
159.49
Relative Abundance
m/z


P204
149.10
205.07
123.30
143.18
130.93
149.62
Relative Abundance
m/z


P264
265.06
178.10
182.94
196.45
95.71
Relative Abundance
m/z


P299
300.74
282.62
299.99
Relative Abundance
m/z

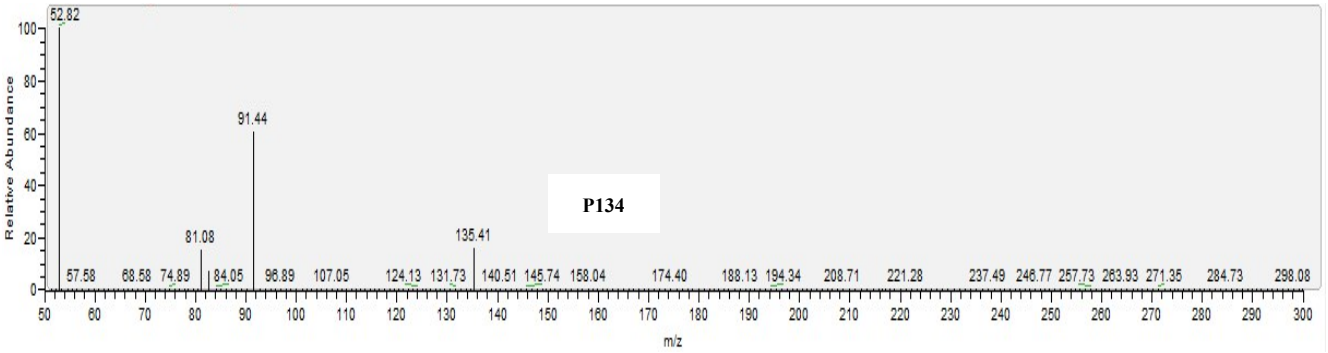


Fig. S4. Mass spectra of NPX and its products.