

## *Supplementary Material*

# **g-C<sub>3</sub>N<sub>4</sub> as photocatalyst for the removal of Metronidazole antibiotic from aqueous matrices under lab and pilot scale conditions**

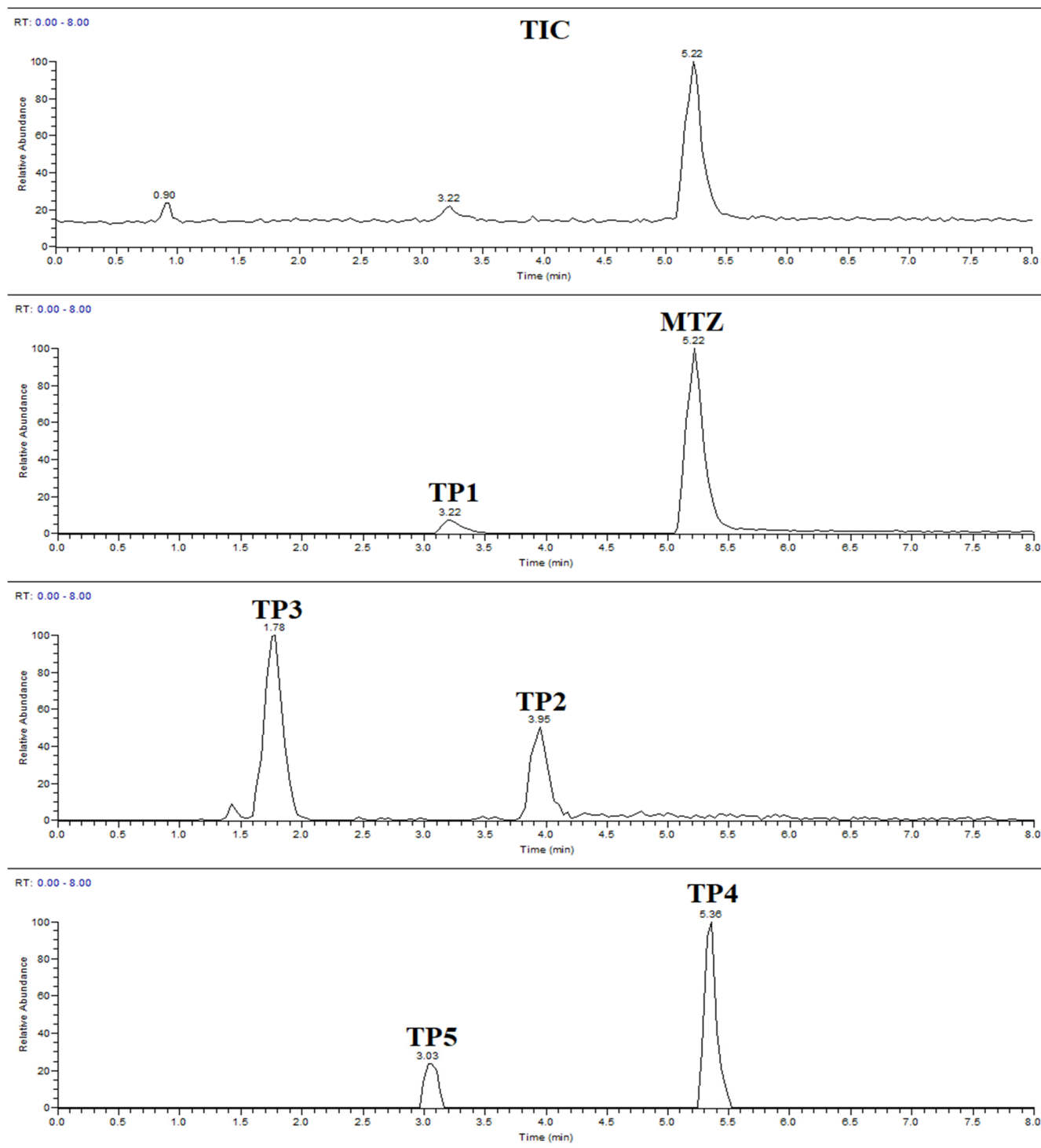
**Christos Lykos<sup>1</sup>, Sotirios Sioulas<sup>1</sup>, Ioannis Konstantinou<sup>1,2\*</sup>**

<sup>1</sup> Department of Chemistry, University of Ioannina, Ioannina, 45110, Greece

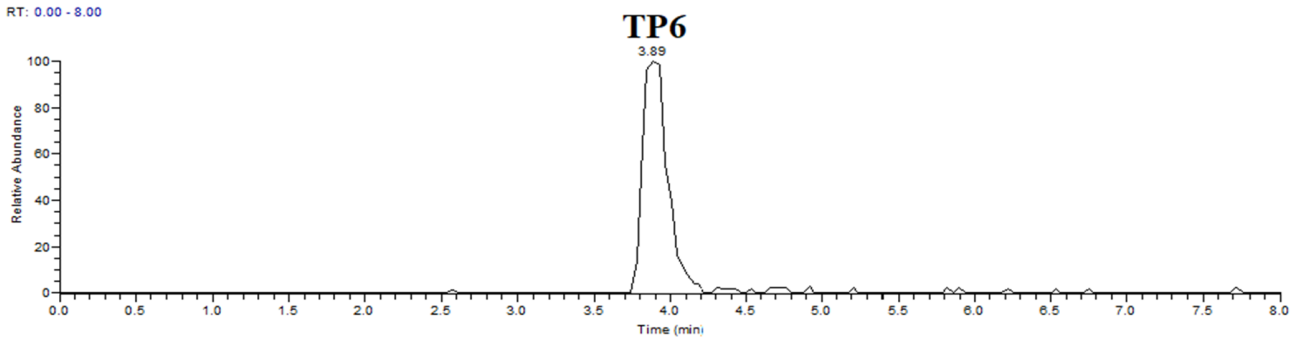
<sup>2</sup> Institute of Environment and Sustainable Development, University Research Center of Ioannina (URCI), Ioannina 45110, Greece

\*Correspondence: iokonst@uoi.gr

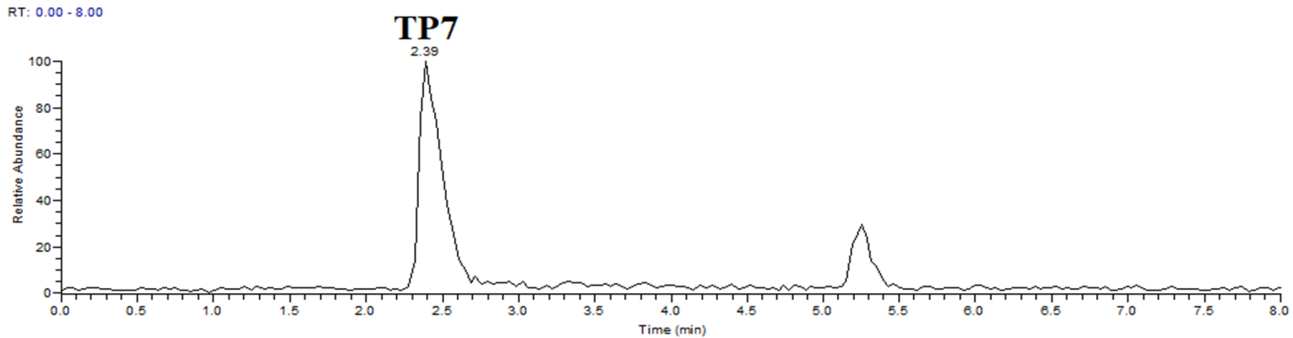
**Figure S1.** Total ion current (TIC) and extracted pseudo-molecular ion  $[M+H]^+$  (EIC) chromatograms of MTZ and its TPs (lab scale conditions).



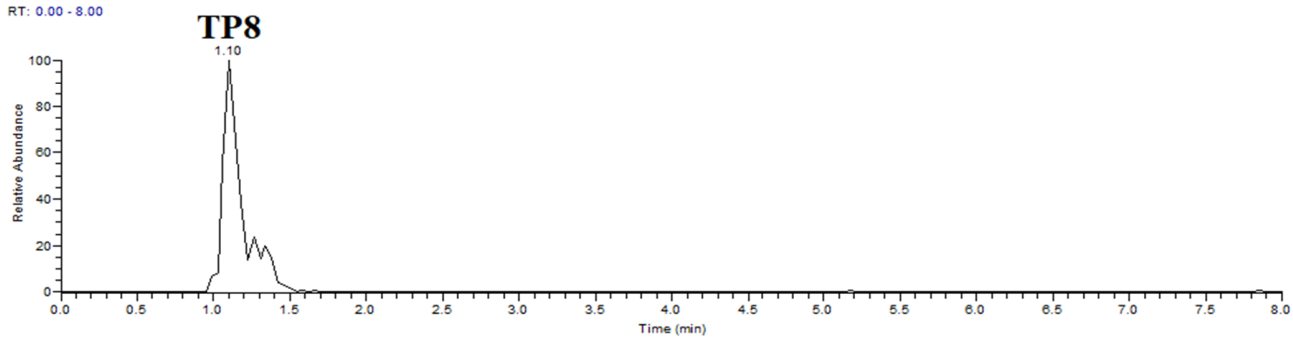
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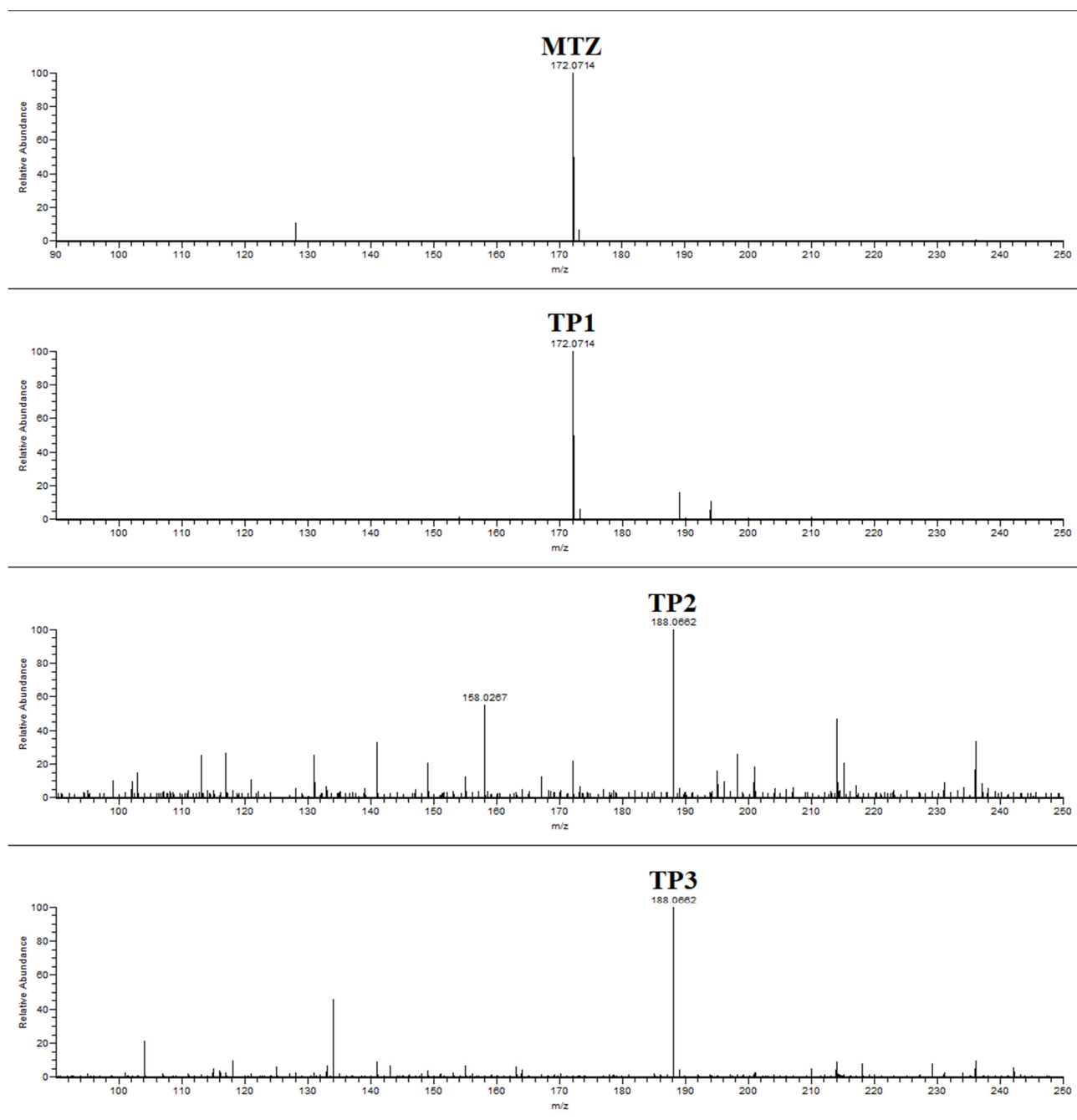
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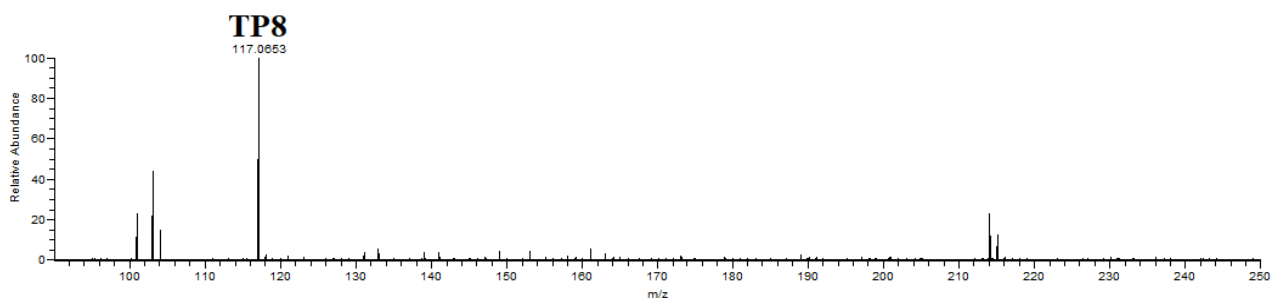
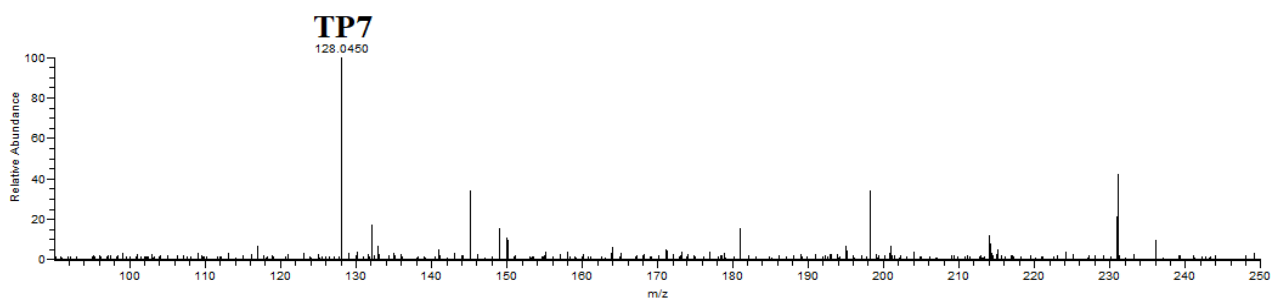
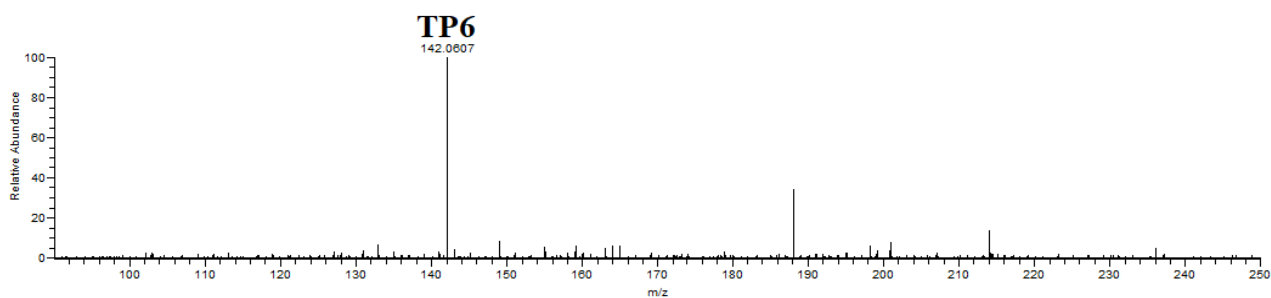
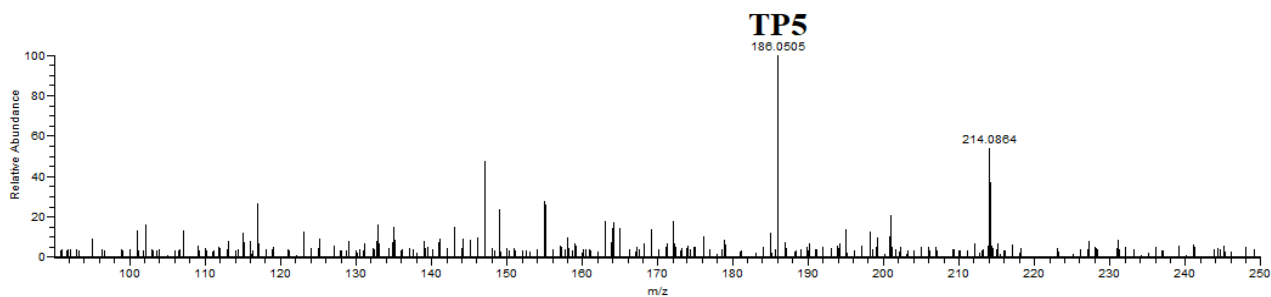
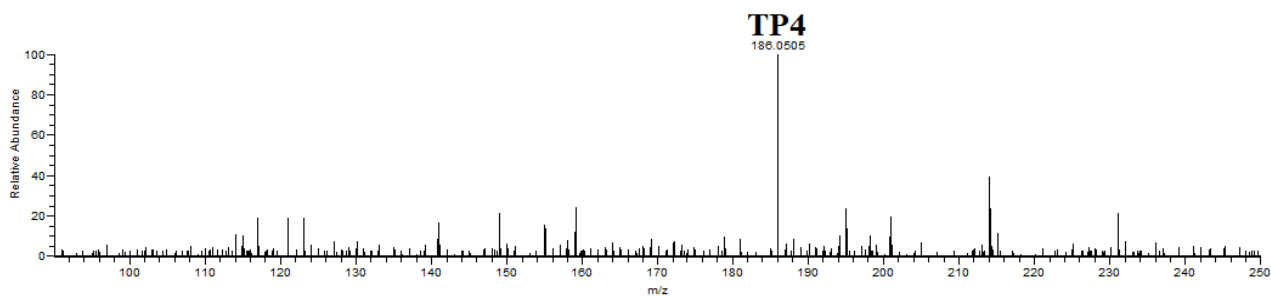


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**Figure S2.** Mass spectra of MTZ and its TPs formed under lab scale conditions





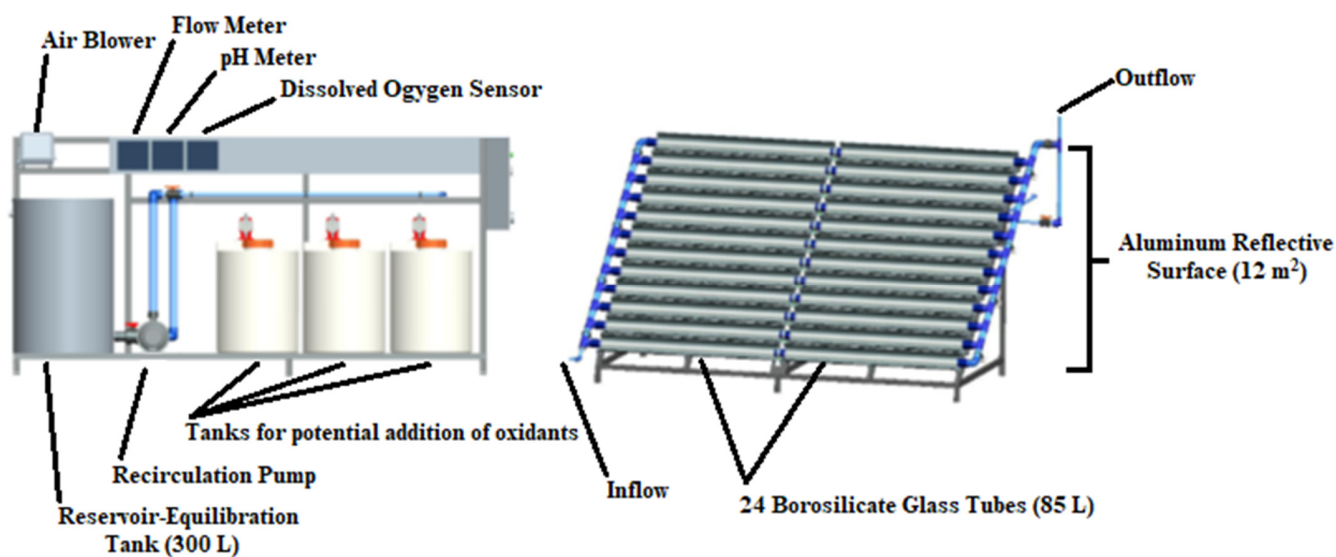
**Table S1.** High resolution mass data of MTZ and its TPs

Compound	t <sub>R</sub> (min)	[M+H] <sup>+</sup> /[M+Na] +	Molecular Formula	Δ (ppm)	RD B	MS <sup>2</sup> /MS <sup>3</sup> [M+H] <sup>+</sup>	Molecular Formula	Δ (ppm)	RD B
MTZ	5.22	172.0714	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> N <sub>3</sub>	-1.846	3.5	MS <sup>2</sup>			
						128.0449	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N <sub>3</sub>	-4.475	3.5
						MS <sup>3</sup>			
TP1	3.22	172.0714	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> N <sub>3</sub>	-1.498	3.5	82.0517	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	-9.991	3.0
						MS <sup>2</sup>			
						154.0606	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> N <sub>3</sub>	-3.330	4.5
						128.0449	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N <sub>3</sub>	-4.475	3.5
						88.0385	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> N	-8.916	1.5
						85.0390	C <sub>3</sub> H <sub>5</sub> ON <sub>2</sub>	-7.636	2.5
TP2	3.95	188.0662	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub> N <sub>3</sub>	-2.033	3.5	MS <sup>3</sup>			
						-			
						MS <sup>2</sup>			
						170.0556	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> N <sub>3</sub>	-2.750	4.5
TP3	1.78	188.0662	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub> N <sub>3</sub>	-2.139	3.5	128.0448	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N <sub>3</sub>	-5.100	3.5
						MS <sup>3</sup>			
						-			
						MS <sup>2</sup>			
						170.0552	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> N <sub>3</sub>	-4.749	4.5
						128.0448	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N <sub>3</sub>	-6.271	3.5
						MS <sup>3</sup>			

						-				
TP4	5.36	186.0505	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub> N <sub>3</sub>	-2.753	4.5	-				
TP5	3.03	186.0505	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub> N <sub>3</sub>	-2.753	4.5	-				
TP6	3.89	142.0607	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> N <sub>3</sub>	-3.119	3.5	MS <sup>2</sup>				
						85.0389	C <sub>3</sub> H <sub>5</sub> ON <sub>2</sub>	-8.459	2.5	
						MS <sup>3</sup>				
						-				
TP7	2.39	128.0450	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N <sub>3</sub>	-3.303	3.5	MS <sup>2</sup>				
						85.0389	C <sub>3</sub> H <sub>5</sub> ON <sub>2</sub>	-7.048	2.5	
						MS <sup>3</sup>				
						-				
TP8	1.10	117.0653	C <sub>4</sub> H <sub>9</sub> O <sub>2</sub> N <sub>2</sub>	-4.306	1.5	MS <sup>2</sup>				
						100.0386	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> N	-7.447	2.5	
						MS <sup>3</sup>				
						-				

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\* tr: retention time, [M+H]<sup>+</sup>/[M+Na]<sup>+</sup>: pseudo-molecular, Δ(ppm): relative mass error, RDB: aromatic ring double bond equivalents



**Scheme S1.** Schematic diagram of the compound parabolic collector (CPC) pilot plant reactor.

**Table S2.** Gradient elution program for the separation MTZ and its TPs.

Analysis Time (min)	Eluent ratio (%)	
	Eluent A	Eluent B
0.0	95	5
2.0	95	5
3.0	90	10
5.0	90	10
10.0	50	50
13.0	95	5
18.0	95	5



**Table S3.** LTQ-Orbitrap instrumentation operational parameters

MS Parameters	Values
Resolution	60000 FWHM
Full Scan	90-600 Da
Mass Tolerance	≤ 5 ppm
Auxiliary Gas Flow	10 a.u.
Sheath Gas	35 a.u.
Spray Voltage	4,0 kV
Collision Energy	35 eV
Capillary Temperature	320 °C
Capillary Voltage	50 V
Tube Lens	90 V