GC-HRMS analysis to evaluate the effectiveness of ozone disinfection for the removal of micropollutants from wastewater

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Appendices

Table A.1. Instrumental conditions for chromatographic separation and data acquisition

Item	**Value**
TRACE 1300 Series GC method	
Splitless time	1 min
Initial Temperature	70º C
Carrier flow	1 mL/ min
Ramp 1	6ºC to 175ºC, hold time 4 min
Ramp 2	3º C to 235ºC, hold time 0 min

Ramp 3	7ºC to 305ºC, hold time 8 min
Q Exactive GC	
Method duration (time)	60 min
Mass tolerance (+/-)	5 ppm
Ionization – Electron energy	70 eV
MS transfer line temperature	280º C
Ion source temperature	260º C
Scan range	70 to 1000 m/z

Text S1 Toxicity test with neonate Daphnia

The methodology used to evaluate the acute toxicity was based on the OECD 202. After extraction, the evaporated extracts were suspended with 0.5 mL of acetone, and then inoculated in a 100 mL glass bottle, allowed to evaporate forming a residue thin layer in the walls. Residues were then suspended again in 50 mL water, heavily vortexed and distributed in two 20 mL vials. To each vial, 10 neonate Daphnia were inoculated. After 48 h, their immobility was monitored (table S1). Mortality responses in the different treatments were compared to those of blank samples using a nested hierarchical ANOVA design with vial nested across replicated treatments.

Table S2 Results obtained for the toxicity test using neonate Daphnia.

	Ozone dose (mg O_3 L^{-1})	**Duplicate**	**Deaths**	**Deaths**	**Total**	**%**	**%**	**Mean**	**SD**
GW	0	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	0 + SPK*	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	3.5	A	0	0	10	0	0	0	0

		B	1	1	10	10	10	10	0
	7.6	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	15.2	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	22.8	A	2	3	10	20	30	25	3.53
		B	2	1	10	20	30	25	3.53
	Blank**	A	0	0	10	0	0	0	0
		B	1	0	10	10	0	5	3.53
UW	0	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	3.5	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	7.6	A	0	0	10	0	0	0	0
		B	2	1	10	20	10	15	3.53
	15.2	A	0	0	10	0	0	0	0
		B	0	0	10	0	0	0	0
	22.8	A	0	0	10	0	0	0	0
		B	3	2	10	30	20	25	3.53
	Blank**	A	1	1	10	10	10	10	0
		B	1	0	10	10	0	5	3.53
	Test control	0	0	10	0	0		0	0

* spiked raw sample

**experimental blanks (extraction procedures)