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Supplementary Material

Efficient removal of diuretic hydrochlorothiazide from water by electro-Fenton process using BDD anode: a kinetic and degradation pathway study

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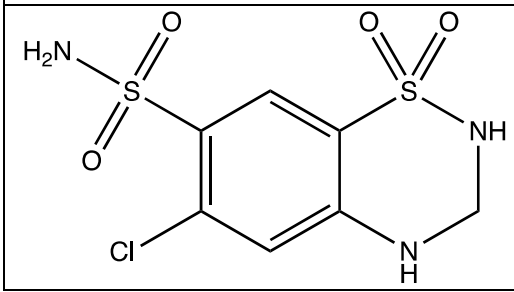
Molecular formula of HCT

The molecular formula of HCT and its pKa value are given in Table S1.

***Table S1**: Hydrochlorothiazide structure and pKa*

Molecule	pKa
	7.9

Intermediates found by GC-MS analysis

The degradation pathway proposed was done thanks to the analysis of the GC-MS spectrum. The small aliphatic compounds were obtained by the chromatography software Xcalibur and the detail is given in Table S2. The bigger molecules were identified thanks to their fragmentation given in Table S3.

***Table S2**: Aliphatic compound found using the following conditions: 1 mM hydrochlorothiazide, 0.1 mM Fe^{2+}, 10 min of electrolysis, extraction with dichloromethane and ethyl acetate, derivatization (BSTFA).*

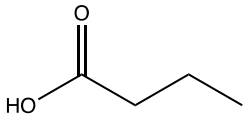
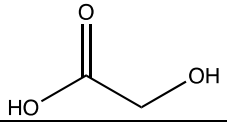
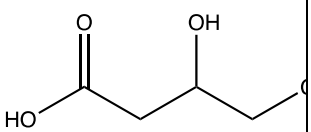
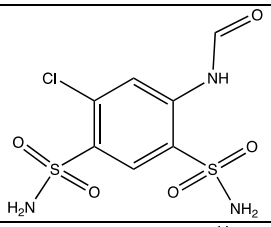
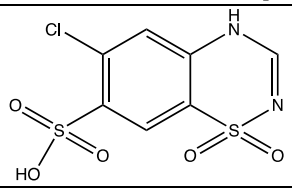
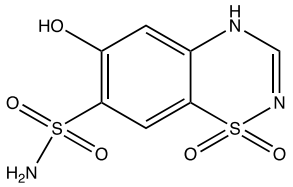
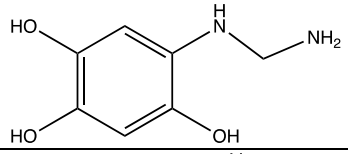
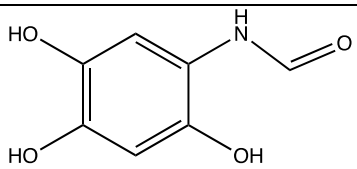
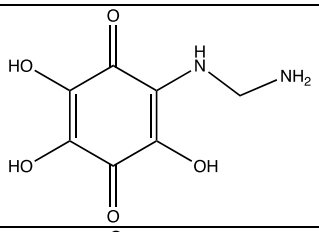
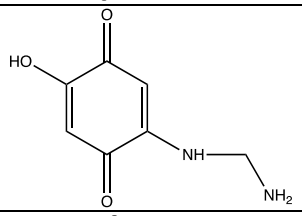
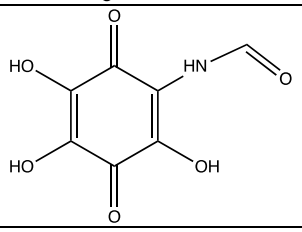
Name	Molecule (without silylation)	Fragmentation	Retention time (min)	Identification letter
Butyric acid		75, 145, 73, 146, 117	4.55	L
2-hydroxyacetic acid		147, 73, 66, 148, 77	6.13	M
3,4-dihydroxybutanoic acid		73, 147, 233, 189, 231	9.55	J

Table S3: *Intermediate compounds found using GC-MS under following conditions: 1 mM hydrochlorothiazide, 0.1 mM Fe^{2+}, 10 min of electrolysis, extraction with dichloromethane and ethyl acetate. The corresponding molecular weight is given in* **red**

Name	Molecule	Fragmentation	Identification letter
N-(5-chloro-2,4-disulfamoylphenyl)formamide		73, **313**,75, 132, 55, 69, 189, 206,285	B
6-chloro-4*H*-benzo[*e*][1,2,4]thiadiazine-7-sulfonic acid 1,1-dioxide		**294**, 199, 296, 93, 141, 213, 201, 279	C
6-hydroxy-4*H*-benzo[*e*][1,2,4]thiadiazine-7-sulfonamide 1,1-dioxide		125, 77, 201, **277**, 157, 175	D
5-hydrazineylbenzene-1,2,4-triol		77, 141, **170**	E
N-(2,4,5-trihydroxyphenyl)formamide		109, 151, 69, 85, 57, 67, **169**	F
2-((aminomethyl)amino)-3,5,6-trihydroxycyclohexa-2,5-diene-1,4-dione		73, 60, 57, 55, 71, 85, 129, 69, 157, 115,171, **200**	G
2-((aminomethyl)amino)-5-hydroxycyclohexa-2,5-diene-1,4-dione		59, 71, 57, 55, 73, 77, 105, 112, 133, **168**	H
N-(2,4,5-trihydroxy-3,6-dioxocyclohexa-1,4-dien-1-yl)formamide		71, 73, 55, 153, 57,69, 60, **199**, 170, 99	I

Formation of NH_4^+ from electro-reduction of NO_3^- during EF treatment

The solutions of 1 mM of NH_4^+ and 1 mM of NO_3^- were electrolyzed using potassium sulfate as electrolyte, under current intensity from 100 to 700 mA with 1 mM of iron (II). Fig. S1 depicts the results obtained. After 8 h electrolysis, the concentration of NH_4^+ is still equal to 1 mM whereas the NO_3^- was transformed into NH_4^+.

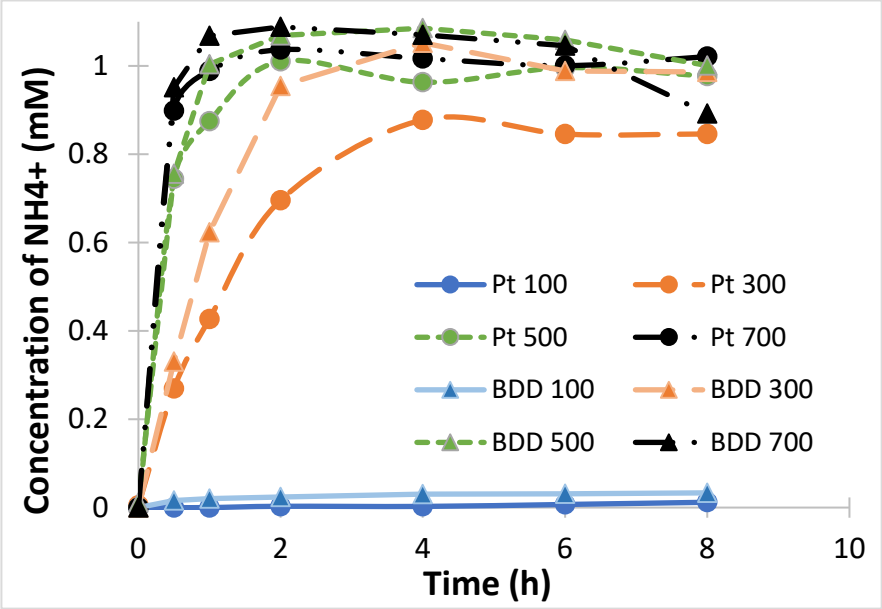


Fig. S1: Evolution of NH_4^+ concentration during EF treatment of 1 mM NO_3^- solution under different currents using BDD or Pt anodes.

Study of the degradation and mineralization with the addition of ions

To consider the effect of the ions present in a real wastewater on the degradation of the HCT, a synthetic solution was prepared by adding different ions. The concentration of ions used was the value of a real wastewater coming from an industrial production of antibiotics. As can be seen in Fig S2 and Fig. S3, there is a slight effect on degradation kinetics but no effect on the mineralization kinetic was observed.

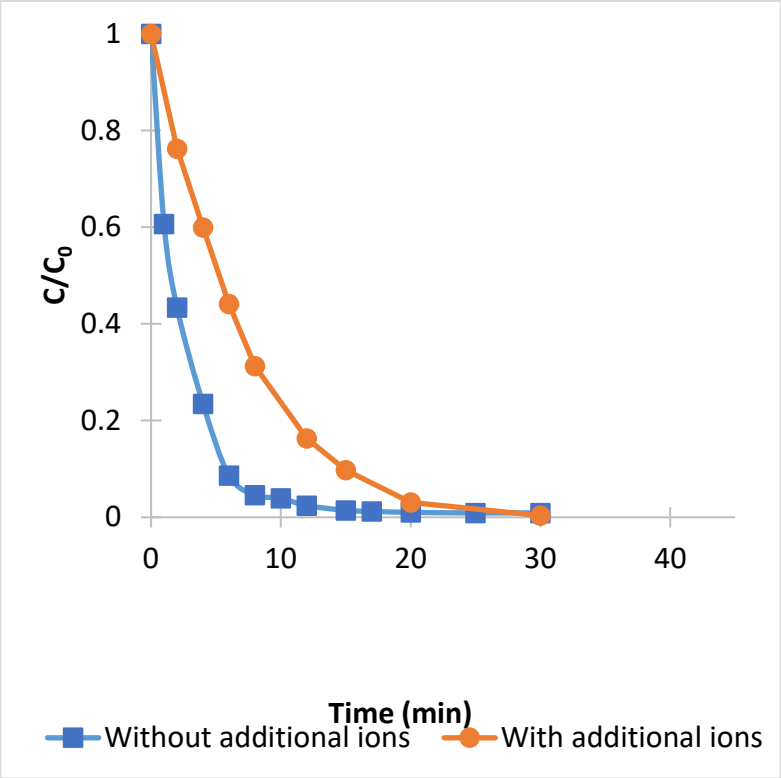


Fig. S2: Kinetic of degradation during the elimination of 0.1 mM HCT solution under 500 mA, 50 mM of Na_2SO_4 and 0.1 mM Fe^{2+} with and without additional ions. The additional ions were 244 mg L^{-1} $NaCO_3$, 48 mg L^{-1} Cl^-, 4 mg.L^{-1} of PO_4^{3-}, 0.9 mg L^{-1} of NO_2^- and 1.5 mg L^{-1} of NO_3^-.

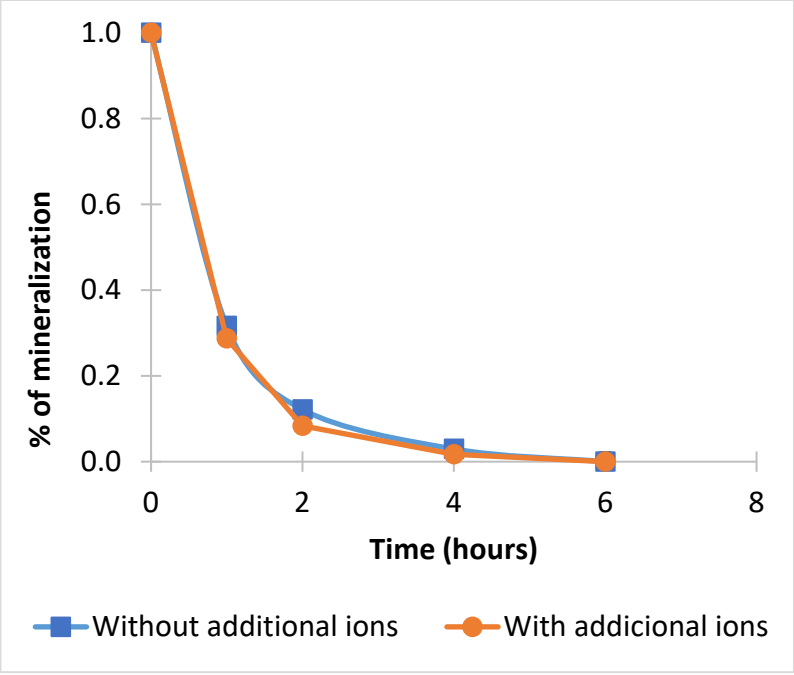


Fig. S3: percentage of mineralization during the degradation of 0.1 mM HCT solution under 500 mA, 50 mM of Na_2SO_4 and 0.1 mM Fe^{2+} with and without additional ions. The additional ions were 244 mg L^{-1} $NaCO_3$, 48 mg L^{-1} Cl^-, 4 mg.L^{-1} of PO_4^{3-}, 0.9 mg L^{-1} of NO_2^- and 1.5 mg L^{-1} of NO_3^-.