Mechanistic study of cefixime degradation with an atmospheric air dielectric barrier discharge – influence of radical scavengers and metal ion catalyst

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Table S1

Physicochemical properties of Cefixime

Parameters	Values
Molecular formula	$C_{16}H_{15}N_5O_7S_2$
Molecular weight	453.5 g/mol
Melting point	218 – 225 ℃
Solubility	Slightly soluble in water, soluble in methanol, sparingly in ethanol but insoluble in ethyl acetate
Colour	White or pale yellow
Density	1.85±0.1 g/cm3
Solubility	55.11 mg/L
pKa	3.53
Stability	Hygroscopic

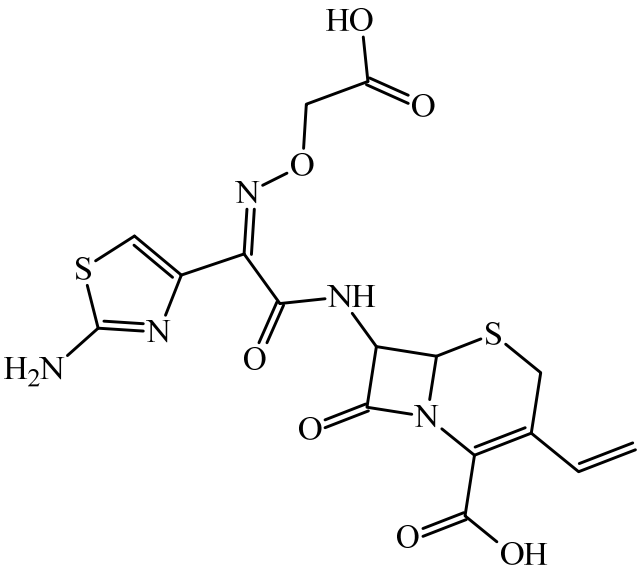
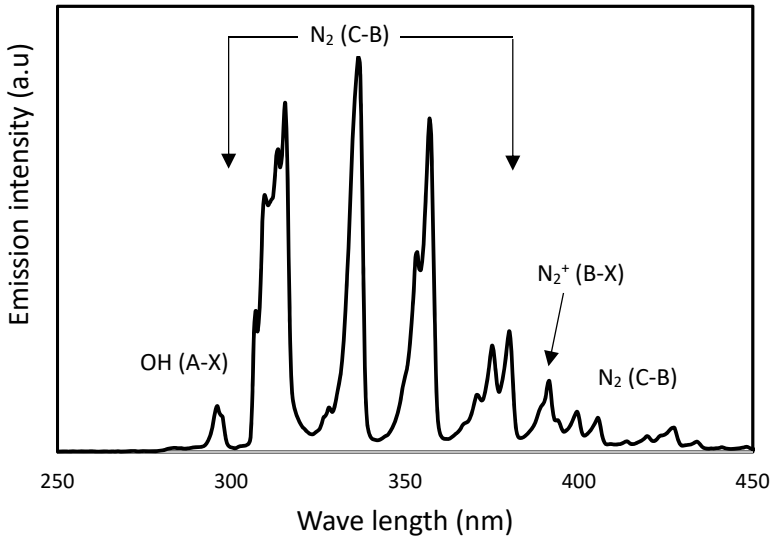
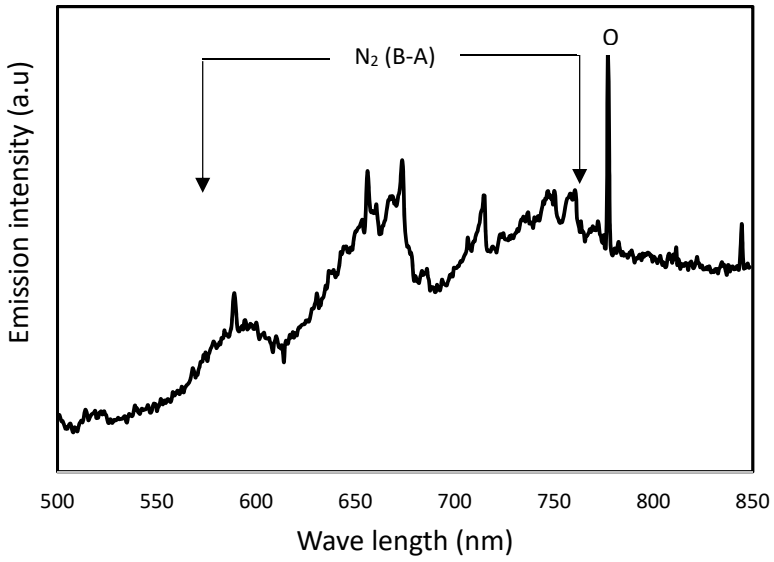


Fig. S1. Molecular structure of Cefixime



(a)



(b)

Fig. S2. Emission spectra from the atmospheric air DBD plasma reactor at 6 kV and 20 kHz. (a) UV spectral range (b) visible/IR spectral range.

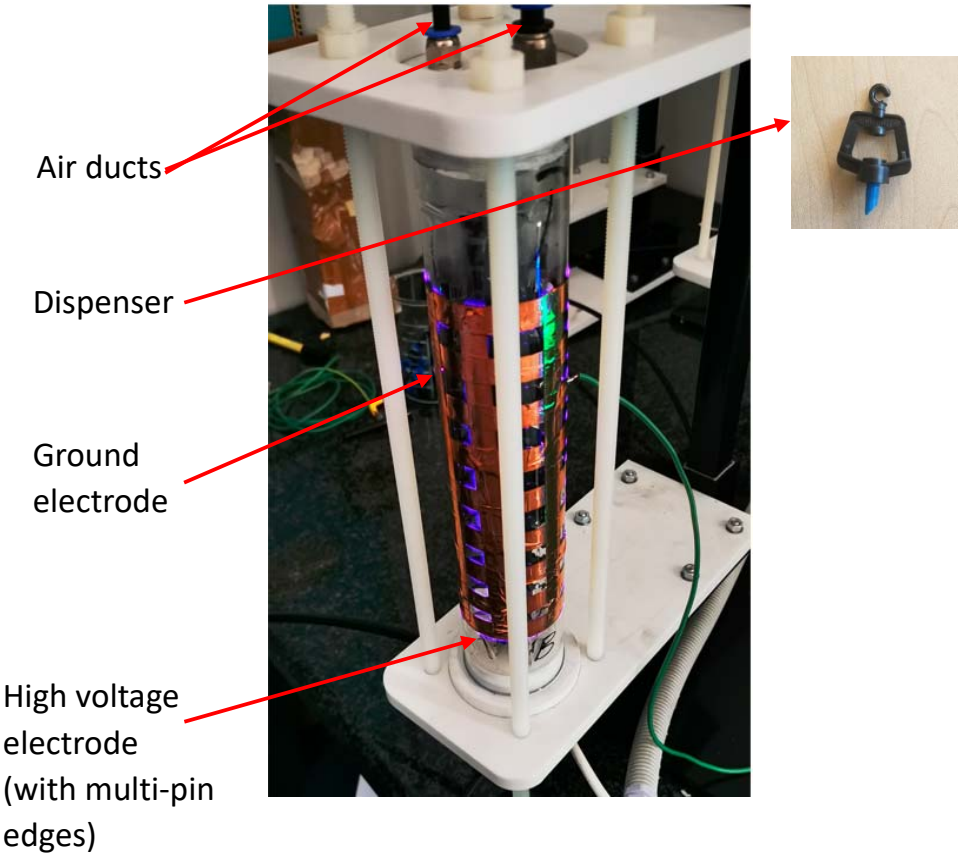


Fig. S3. A picture of the DBD plasma reactor

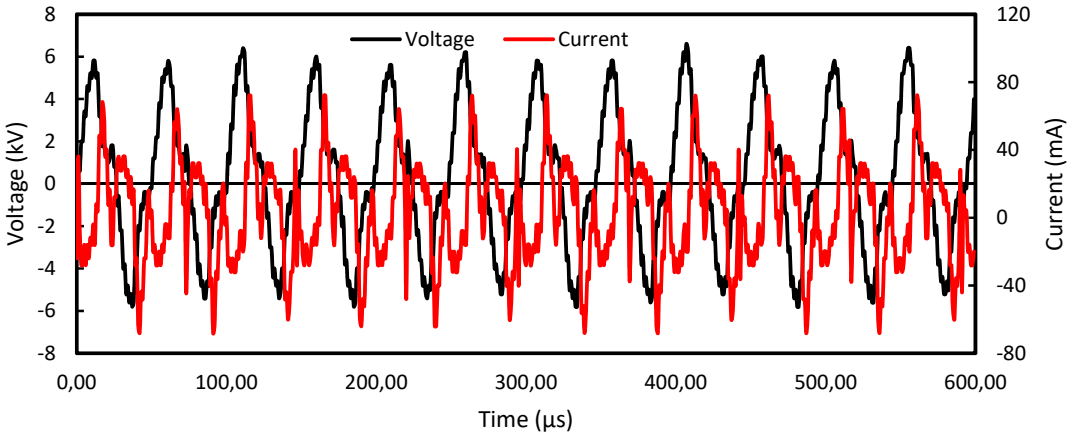
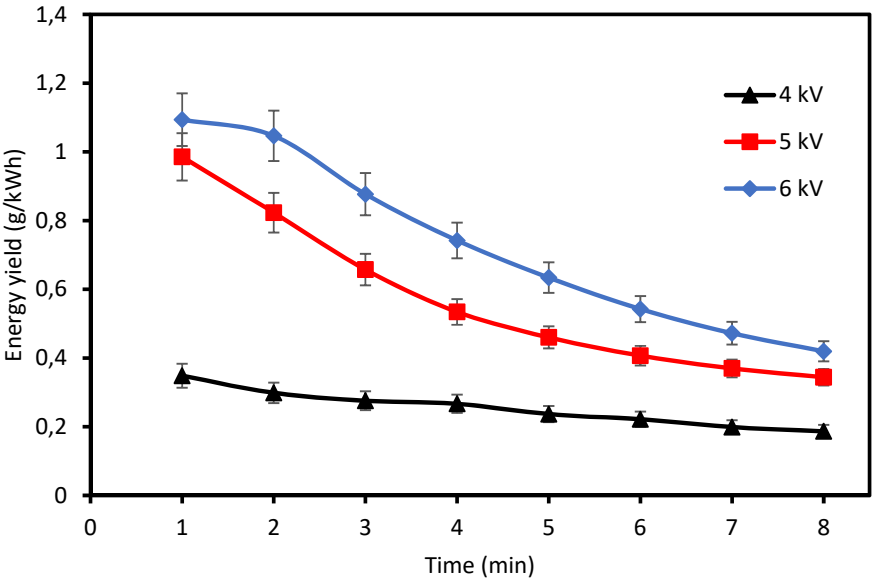
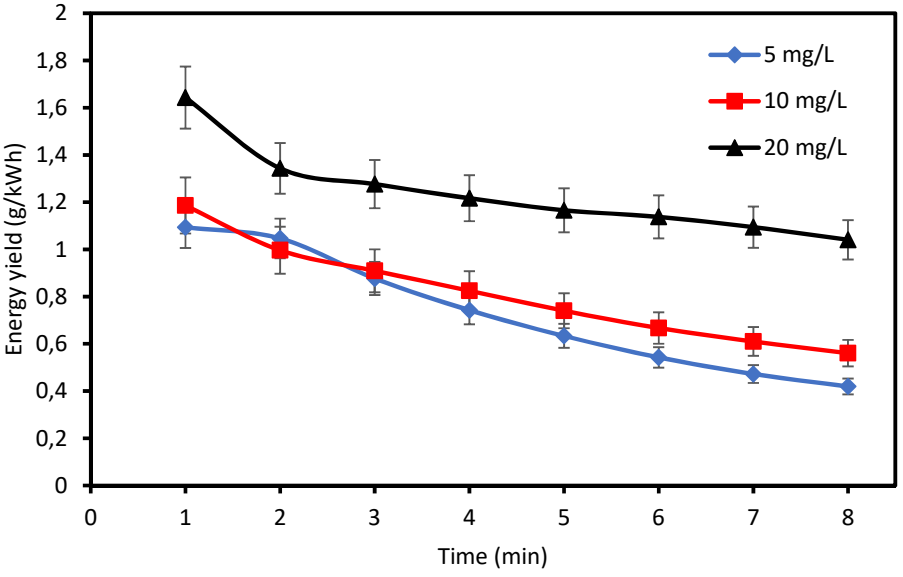


Fig. S4. Representation of the current and voltage waveforms recorded at 6 kV and 20 kHz voltage and frequency, respectively.

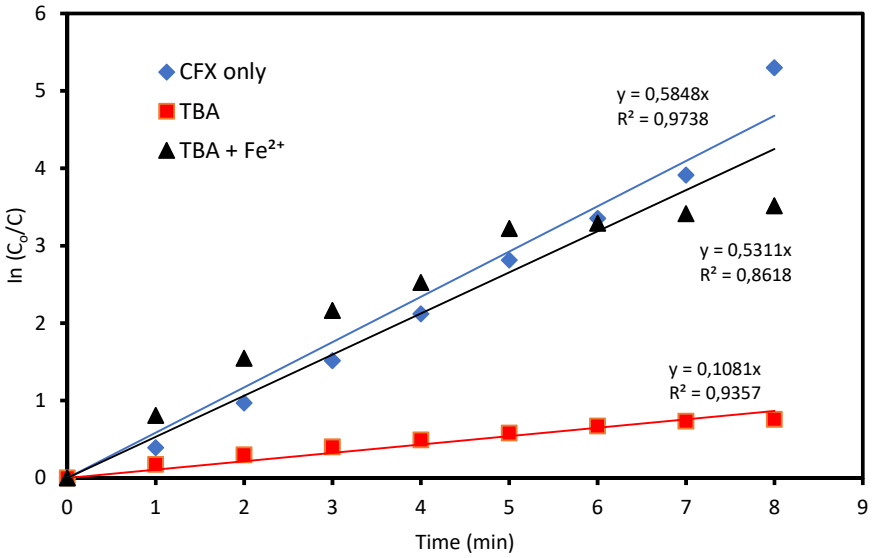


(a)

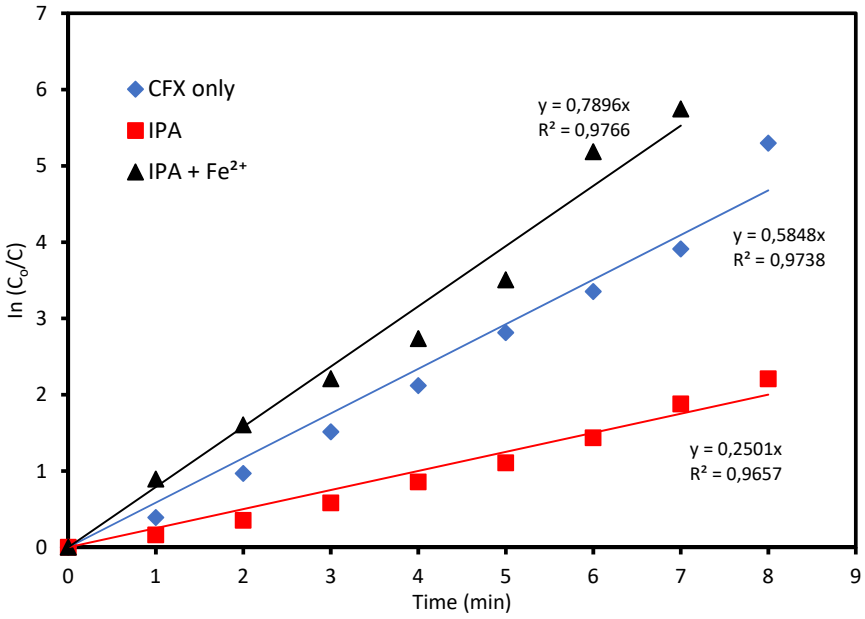


(b)

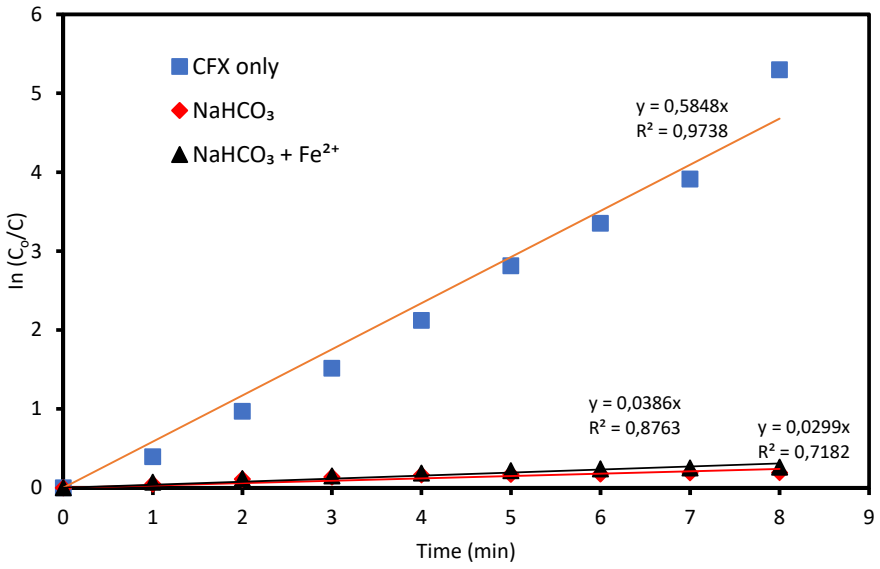
Fig. S5. Energy yield comparison (a) Voltage (b) Initial concentration


CFX only
TBA
TBA + Fe²⁺
y = 0,5848x
R² = 0,9738
y = 0,5311x
R² = 0,8618
y = 0,1081x
R² = 0,9357
ln (C₀/C)
Time (min)

(a)


CFX only
IPA
IPA + Fe²⁺
y = 0,7896x
R² = 0,9766
y = 0,5848x
R² = 0,9738
y = 0,2501x
R² = 0,9657
ln (C₀/C)
Time (min)

(b)

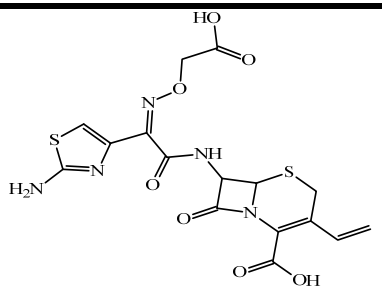
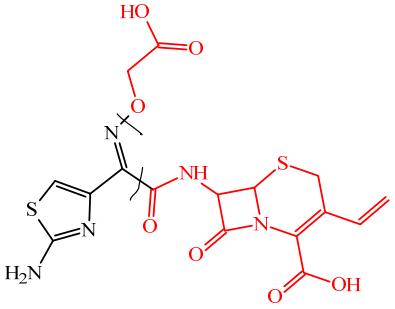


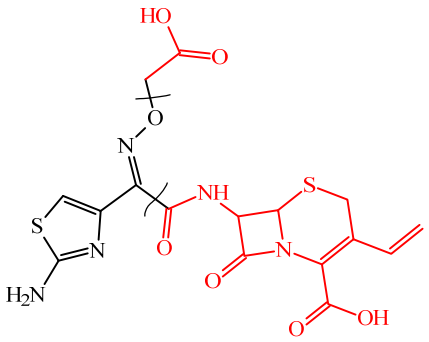
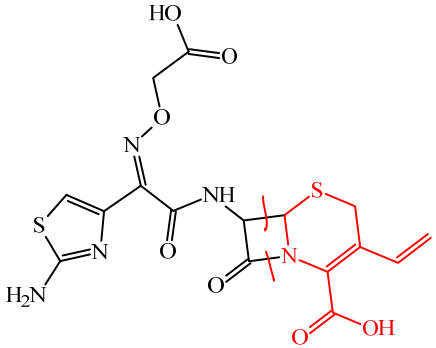
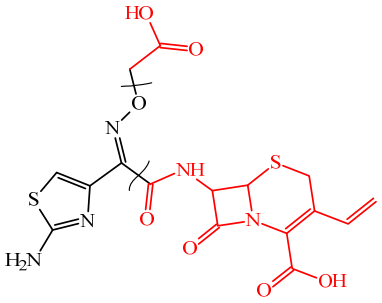
(c)

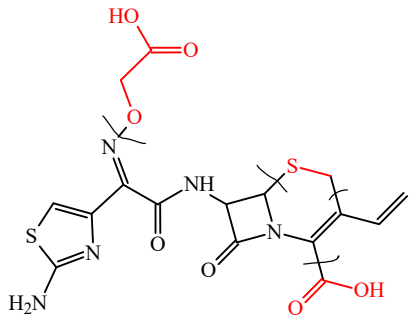
Fig. S6: Rate of reaction observed at the different additives (a) TBA (b) IPA (c) $NaHCO_3$

Table S2

Degradation byproducts for cefixime with the DBD plasma reactor

Identity	Name of identified degradation products	Chemical formula	Rt (min)	Characteristic ions (m/z)	Suggested structure	Exact mass	Theoretical mass
C1	Cefixime	$C_{16}H_{15}N_5O_7S_2$	3.55	454.0501		453.0413	
C2	5-[(E)-Hydrazonomethyl]-1,3-thiazole	$C_4H_5N_3S$	0.80	128.0234		127.0204	127.0137

C3	1,3-Thiazole-4-carbohydrazine	$C_4H_6N_3OS$	0.93	144.1028		144.0232	144.0284
C4	1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxopurine-7-ethanesulfonate	$C_9H_{11}N_4O_5S$	1.06	287.0466		287.0450	287.0381
C5	ethyl N-(oxomethyl)carbamate	$C_4H_6NO_3$	3.28	116.0918		116.0348	116.0318

C6	4-Amino-5-cyano-2-methylthio-6-(3-nitrophenyl)-pyrimidine	$C_{12}H_{10}N_5O_2S$	5.56	288.2913		288.0555	288.0484

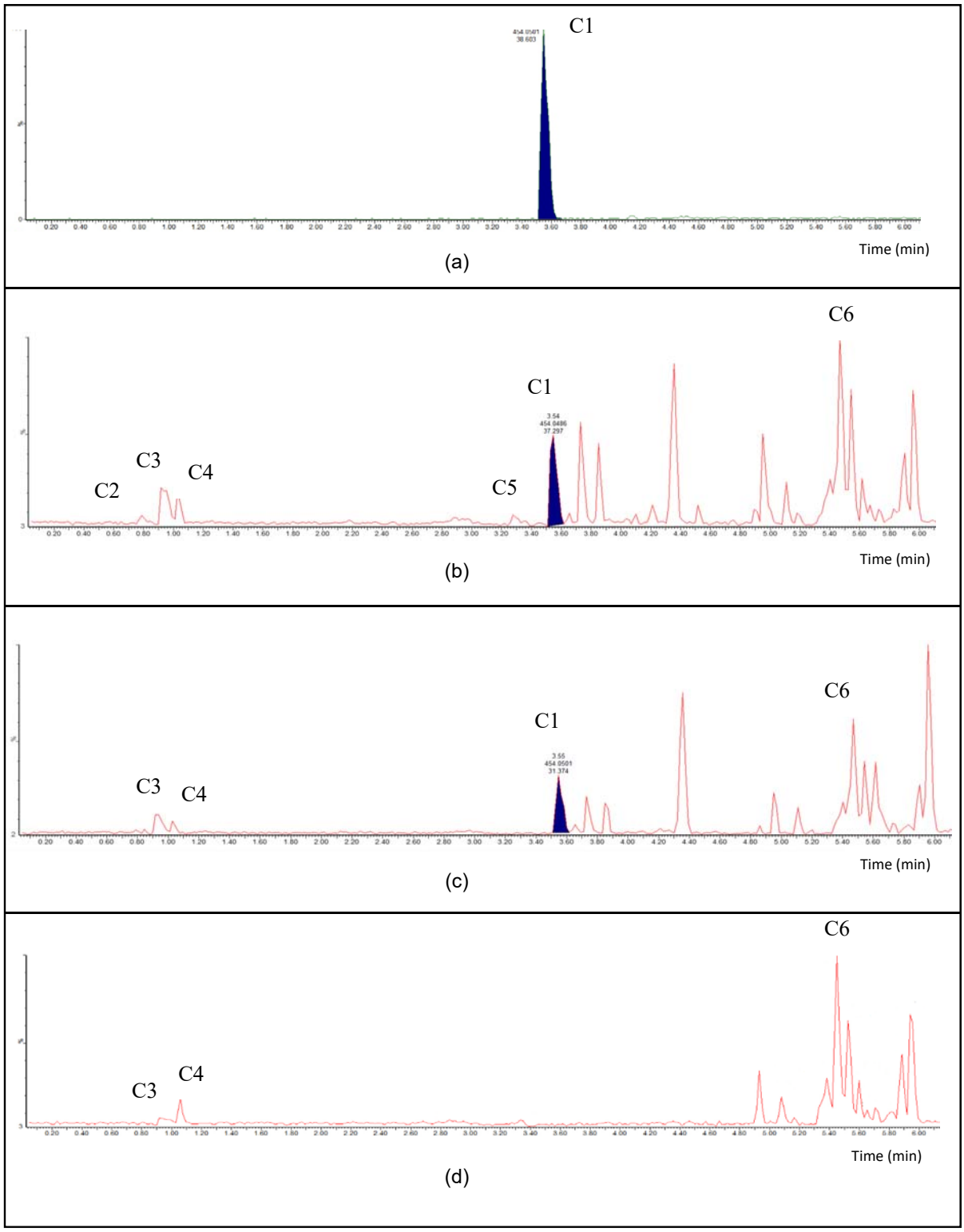


Fig. S7: Chromatograms for the degraded CFX with the DBD plasma reactor at different time intervals (a) pure CFX (b) 1 min (c) 2 min (d) 8 min

The toxicity of individual intermediates is often difficult to be detected directly. Using the ChemSpider Search and share chemistry, the name of the intermediates or transformation products (TPs) in relation to the proposed structure of the TPs obtained using the accurate masses approach on the quadrupole time-of-flight (q-TOF-LCMS) mass spectrum analysis. After obtaining the name of the TPs, their toxicity was predicted by the Toxicity Estimation Software Tool (T.E.S.T.) Version 5.1.1. The authors used different Endpoints and Methods under the calculation options. For example, the 48-hour *Tetrahymena pyriformis* IGC50 was checked for all the TPs while using the Consensus method under the Quantitative Structure Activity Relationships (QSARs) methodologies.

Screenshots are presented for the primary compound, Cefixime and one of the TPs (5-[(E)-Hydrazonomethyl]-1,3-thiazole) using the *Daphnia magna* LC50 (48 hr) Endpoint and the Consensus method for the predictions below:

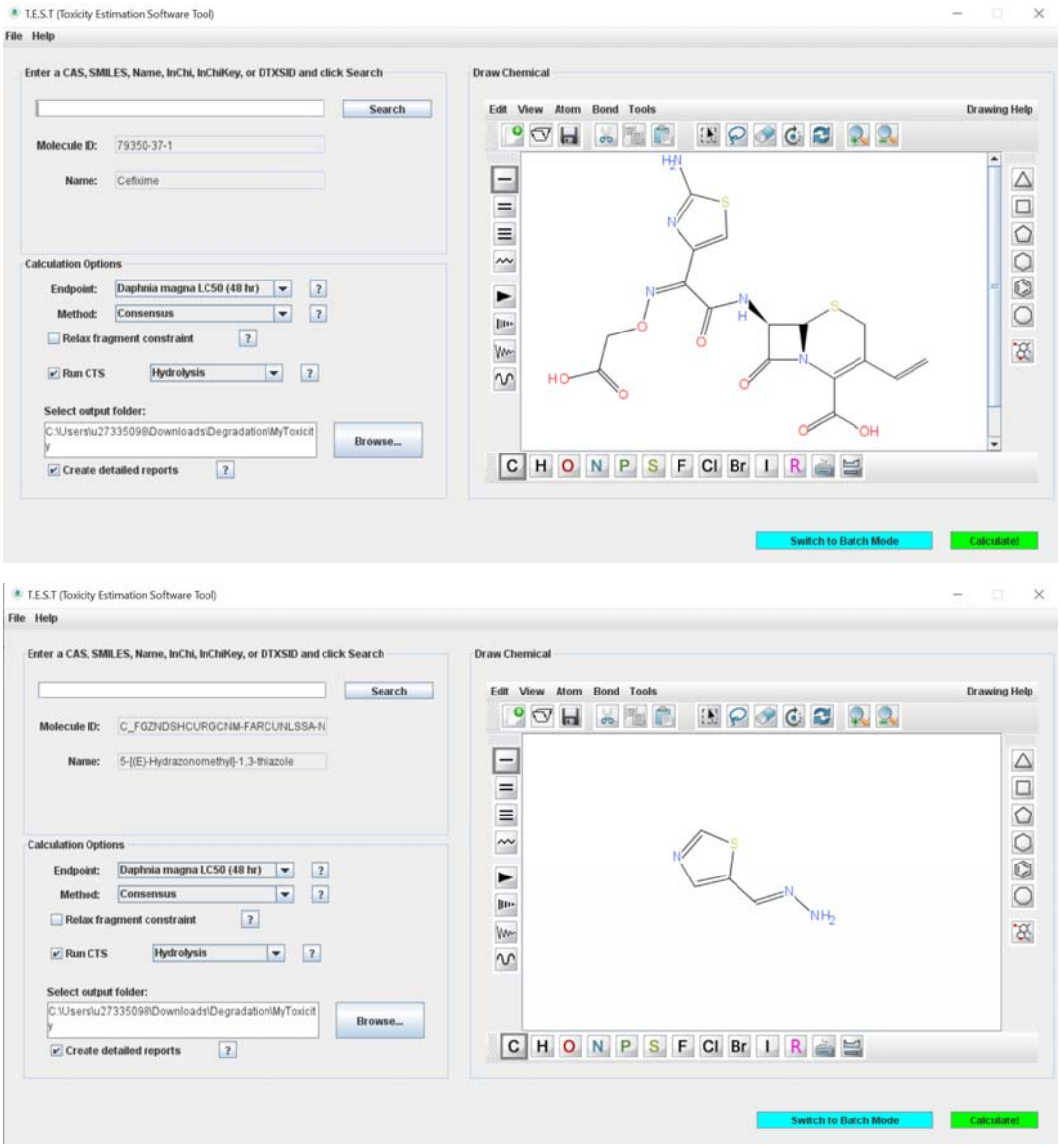


Fig. S8: Screenshots of Cefixime and one of the transformation compounds (5-[(E)-Hydrazonomethyl]-1,3-thiazole) using the *Daphnia magna* LC50 (48 hr) Endpoint and the Consensus method in T.E.S.T

Table S3

Acute and chronic toxicity of Cefixime and its transformation products predicted using T.E.S.T version 5.1.1.

	Consensus method			**Hierarchical clustering method**		
Compound	Fathead minnow (96 hr) - LC_{50} -Log 10 (mol/L)	*Daphnia magna* (48 hr) - LC_{50} -Log 10 (mol/L)	*Tetrahymena pyriformis* (48 hr)-IGC_{50} -Log 10 (mol/L)	Fathead minnow (96 hr) - LC_{50} -Log 10 (mol/L)	*Daphnia magna* (48 hr) - LC_{50} -Log 10 (mol/L)	*Tetrahymena pyriformis* (48 hr)-IGC_{50} -Log 10 (mol/L)
C1 - CFX	N/A*	2.70	N/A*	N/A*	2.40	N/A*
C2	N/A+	4.41	N/A*	N/A+	5.27	N/A*
C3	N/A**	N/A**	N/A**	N/A**	N/A**	N/A**
C4	2.43	N/A+	N/A+	1.90	N/A+	N/A+
C5	2.68	3.02	N/A*	2.97	3.02	N/A*
C6	5.52	5.68	4.52	5.77	5.78	4.50

LC50 means Lethal Concentration 50.

IGC50 means Growth Inhibition Concentration 50.

* The consensus prediction for this chemical is considered unreliable since only one prediction can only be made

+ No prediction can be made

** Transformation Compound - 1,3-Thiazole-4-carbohydrazine is not found