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

Values		
C ₁₆ H ₁₅ N ₅ O ₇ S ₂		
453.5 g/mol		
218 – 225 °C		
Slightly soluble in water, soluble in methanol,		
sparingly in ethanol but insoluble in ethyl		
acetate		
White or pale yellow		
1.85±0.1 g/cm3		
55.11 mg/L		
3.53		
Hygroscopic		

Physicochemical properties of Cefixime



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.





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



(a)





Fig. S6: Rate of reaction observed at the different additives (a) TBA (b) IPA (c) NaHCO3

Table S2

Identity Name of identified Rt Suggested structure Theoretical mass Chemical Characteristic Exact mass degradation products formula (min) ions (m/z) C1 453.0413 Cefixime $C_{16}H_{15}N_5O_7S_2$ 3.55 454.0501 HO H_2 ΟН C2 5-[(E)- $C_4H_5N_3S$ 0.80 128.0234 HO 127.0204 127.0137 Hydrazonomethyl]-1,3-thiazole H_2N 0

Degradation byproducts for cefixime with the DBD plasma reactor







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:

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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)-IGC₅₀ -Log 10 (mol/L)	Fathead minnow (96 hr) - LC₅₀ -Log 10 (mol/L)	Daphnia magna (48 hr) - LC₅₀ -Log 10 (mol/L)	Tetrahymena pyriformis (48 hr)-IGC₅₀ -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