OXIDATION OF PHENOTHIAZINE-DERIVED PHARMACEUTICALS BY FERRATE(VI): AN ASSESSMENT OF TRANSFORMATION PRODUCTS AND BIODEGRADABILITY

OTA – S01

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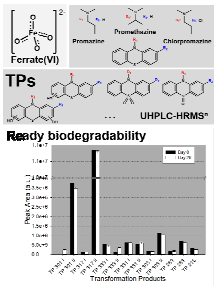
INTRODUCTION

Pharmaceuticals are established as micro-pollutants [1]. Drinking water treatment plants cannot completely eliminate these kind of contaminants [2]. Potassium ferrate (K_2FeO_4) has an oxidizing-coagulant character in a single process [3]. However, incomplete mineralization lead to transformation products (TPs). TPs are new substances which might have similar and non-target interactions in the environment [4].

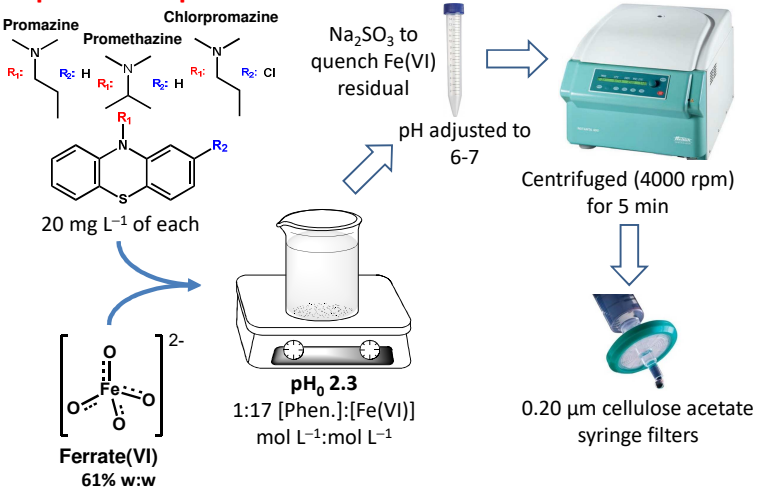
Phenothiazine-derived drugs are worldwide prescribed as first-generation antipsychotic, antiparkinson and antihistamines. Chlorpromazine, Promazine, Promethazine are among the most used phenothiazine-derived pharmaceuticals.



METHODOLOGY

- K_2FeO_4 (61% w:w) was prepared according to Delaude and Laszlo (1996) [5].

Experimental procedure



Monitoring, elucidation and proposal of TPs

UHPLC-LTQ-Orbitrap-XL MS
High-resolution mass spectrometer (HRMS)
H-ESI ion source
Positive ion mode
Non-target approach MS^n mode
CID 25-27 V

Column C18 ec RP18 CC 125-2 mm Nucleodur 100-3

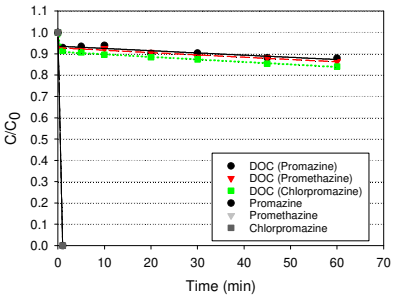
Ready biodegradability (OECD 301 D)

	Blank	Quality Control	Substance Tested	Toxicity Control
Mineral medium	x	x	x	x
Inoculum (2 drops L^{-1})	x	x	x	x
Sample (ThOD 5 mg L^{-1})	–	–	x	x
Sodium acetate (ThOD = 5 mg L^{-1})	–	x	–	x

- Low amount of nutrient, Low bacterial density.
- 20 ± 1 ° C in the dark for 28 days

RESULTS AND DISCUSSION

Primary elimination and mineralization



Kinetic of mineralization

Two steps of pseudo-first order

$C_t = C_1 e^{-k_{1obs}t} + C_2 e^{-k_{2obs}t}$

$PRO_t = 0.0643e^{-147.88t} + 0.9357e^{-0.0012t}$
r^2 0.953 ($p < 0.05$)

$PRM_t = 0.0721e^{-27.36t} + 0.93e^{-0.0012t}$
r^2 0.983 ($p < 0.05$)

$CPR_t = 0.0901e^{-2.7189t} + 0.91e^{-0.0014t}$
r^2 0.998 ($p < 0.05$)

Figure 1. Mineralization of PRO, PRO and CPR by Fe(VI) oxidation-coagulation process. Initial conditions: [PRO]/[PRM]/[CPR] 20 mg L^{-1}, pH 2.3, 1:17 mol L^{-1}: mol L^{-1} [Phen]:[Fe(VI)] ratio, and temp.: 20 ± 2 °C.

Proposal of degradation pathway

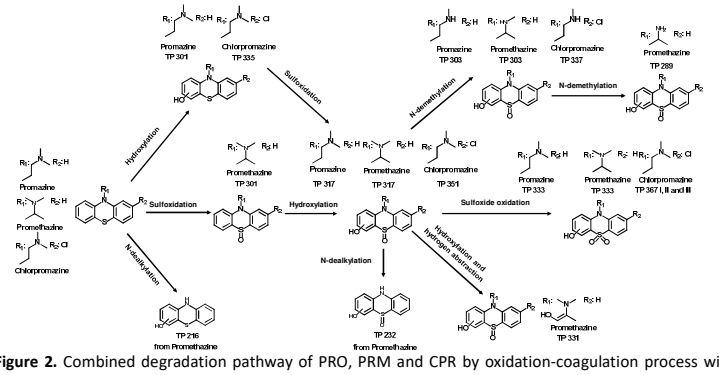


Figure 2. Combined degradation pathway of PRO, PRM and CPR by oxidation-coagulation process with Fe(VI).

Aerobic biodegradation results (OECD 301 D)

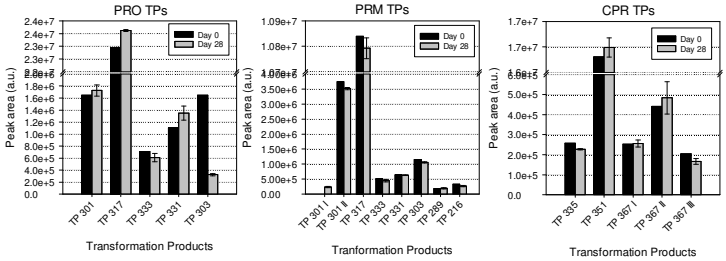


Figure 3. Peak areas of the transformation Products (TPs) formed from PRO, PRM, and CPR through Fe(VI) oxidation before and after 28 days of Closed Bottle Test (CBT).

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