Simulation of the redox metabolism of antidepressant active compounds (emerging pollutants) by Electrochemistry/Mass spectrometry (EC/MS).

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Description / Background
The aim of this project was to study the metabolic pathways and fate of various emerging pollutants in the environment, where they could cause acute or chronic effects to wildlife. Despite the numerous reports in environmental occurrence of emerging pharmaceutical pollutants, even at extremely low concentrations, their environmental significance pertaining to environmental effects is largely unknown.

The project focused on the oxidative and reductive metabolic pathways of selected compounds, mainly antipsychotic pharmaceuticals such as haloperidol, fluoxetine, diazepam and chlorpromazine. The ROXY™ system provides this capability with a special series of electrodes and with two different reactive cells coupled with either iontrap MS or TOF MS. The main parameters studied, were the presence of various matrices (TOC, humic substances), pH values and different initial concentrations of pollutants.

Experimental
Large electrochemical cell PrepCell™ (fig 1)
Small scale ReactorCell ™ (fig 2)
Flowrate: 19/55L/min respectively
Rate of potential ramp: 20mV/sec

Electrodes tested
• MagicDiamond MD
• Glassy Carbon GC
• SS reduction (Ti-based)
• Au
• Pt

PARAMETERS TESTED
• Buffer system ammonium formate 10mM / ACN 50:50
• pH 4, 5, 6, 7, 8, 10
• Various TOC concentrations
• Simulated groundwater, simulated wastewater and real wastewater

Application of various voltages and byproduct formation
*“steps” on the voltamogram indicate oxidative changes
• Haloperidol (MD), pH = 7 buffer 50:50 NH4CHO

Fate and mechanism of Haloperidol transformations

Conclusions
- Electrochemistry MS provides a useful tool for the simulation of environmental transformations of pollutants
- More that 10 by products are formed for haloperidol, 4 of them are naturally produced in the human liver
- The effect of pH shows a slight increase of by product formation at lower pH
- Magic Diamond seems to be the best option for its wide voltage range, high water protolysis potential, robustness and longer lifetime.
- Matrix seems to affect the number of produced by products and the intensity of the initially produced. Humic acid acts inhibitory, probably due to adsorption and antagonistic phenomena.

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