Rapid Mimicking of Drug Metabolism by Electrochemistry-MS

1. Objective

Using Electrochemistry-MS (EC-MS) as an alternative tool to enzymatic CP540 reactions in (drug) metabolism: Rapid, enzyme-free free metabolism.

2. Introduction

The knowledge of the metabolic pathways and the bio-transportation of new drugs are crucial for elucidation of degradation routes of the new drug compounds, especially in the area of possible toxicity. In-vitro studies are based on incubating drug candidates with, e.g., liver cells (microsomes) and isolating and detecting the metabolic products. With the availability of the ROXY™ Electrochemistry-MS (EC-MS) system oxidative metabolism, which usually occurs in the liver cells by Cytochrome P450 oxidation, can be mimicked successfully within seconds and detected by mass spectrometry. Combining EC with MS creates a powerful platform for oxidative metabolism and overcomes some of the laborious tasks such as isolating the metabolites in vivo, e.g., urine, plasma, or in-vitro studies, etc., microsomes.

For more information, visit our booth #614

3. Instrumentation

3.1. Oxidative Metabolism (Phase I)

3.2. Adduct Formation (Phase II)

4. Results

5. Publications using ROXY™ EC to mimic drug metabolism (since 2017)

Outlines of 4-hiproquinoxaline in Aposphage Solutions as a Model for Exteriorisation of Fumaric into EC

Online Monitoring of Methanol Electro-Reduction Reactions by Ambient Mass Spectrometry

High Resolution Mass Spectrometry to Study Oxidation Products of Trimethoprim

Preparation of the Key Metabolite of Trimethoprim by a Specific Electrochemical Method

Structural characterization of electrochemically and in vivo generated potential metabolites of selected insecticides

Characterization of the Reaction Products of 4-Hydroxyestradiol with a Pd Electrode

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Studying the effect of bi-directional Pd/H 2 electrodes on electrochemical reactions

Early detection of in vivo formed acetaminophen metabolites using an electrochemical flow cell and a high resolution mass spectrometer

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Structure of Nucleic Acids by Mass Spectrometry

Presence of Caffeine in Human Tissue Using Electrochemical Flow Cell-Mass Spectrometry

Electrochemical Cytosine DNA-Modification Detection

Electrochemical Metabolism of Breast Cancer: A New Approach for Early Detection

Electrochemical Determination of the Oxidation Products of Phenobarbital

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