Electrochemistry vs. in-vitro:

- seconds vs. weeks
- no isolation/clean-up
- phase I and II metabolism
- complementary to in vivo
- saving rodents (rats, mice)

Methods / Instrumentation

An analytical and preparative electrochemical cell (Antec) equipped with a glassy carbon (GC) or conductive diamond (MD) working electrode were used for the oxidation of drug compounds. The cell potential was ramped from 0 to 2V (GC) or to 3.5 V (MD) during the experiments. The outlet of the electrochemical cell was connected directly to the electrospray source of a MicroTOF-Q (Bruker Daltonics, Germany). Typically 10 µM solutions in ammonium formate (acetate)/acetonitrile are pumped through the electrochemical cell at a flow rate of 10—50 µL/min. For the formation of GSH adducts, 50 – 100 µM GSH was added after the EC cell.

Results

Amodiaquine was chosen as model drug to investigate oxidative metabolism using the ROXY EC System dedicated for single component screening. Electrochemical conversion of the amodiaquine into reactive phase I metabolites and their GSH conjugates were successfully achieved.

References

[1] Lohmann W. et al., LC-GC Europe January (2010) 1