Antec Scientific

Reference List Electrochemistry-MS (EC-MS)

Compendium of >130 publications using the ROXY EC System

ROXY reference list #210_016_06

Design: MGO-studio, Maarssen, NL
Illustrations: Antec Scientific

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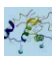
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Electrochemistry - Mass Spectrometry (EC–MS)

Why?

Over 90% of the world's existing compounds possess REDOX properties making them either oxidizable or reducible. By injecting your analyte into an electrochemical cell and identifying the reaction products by MS, many of nature's REDOX reactions can be mimicked (simulated) within seconds without any biological interactions, making on-line EC-MS the technique of choice.

Electrochemistry-MS the technique of choice for fast simulation of any REDOX reactions!

In-electro a much faster and cleaner alternative to costly and time consuming *in-vivo, in-vitro*, microbial, enzymatic or chemical reactions.

When?

EC-MS is the perfect analytical technique for:

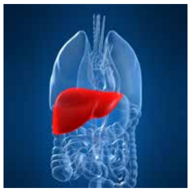
- Fast generation of (drug)metabolites, intermediates and degradants
- No interferences with matrix (e.g., cell membranes, microsomes)
- No need of costly enzymes
- Direct identification of reaction products including short lived components
- Substantial time and cost savings compared to chemical or enzymatic reactions
- Superior MS data: better Id and sequence coverage
- Easy scale-up for synthesis of mg quantities

Typical application are in proteomics, drug metabolism, environmental degradation, drug stability testing, and electrochemical synthesis to name the most prominent.

Where?

Proteomics

In proteomics and protein chemistry Electrochemistry (EC) is mainly used for the **reduction of disulfide bonds**, thereby replacing the use of the often harsh and insufficient chemical reduction (DTT, TCEP). The reduction is instantaneously to allow its on-line integration into the HDX-MS, top-down and recently also in bottom-up LC-MS workflows. Superior characterization of proteins/ peptides including immunotherapeutics (mAbs) has been published.

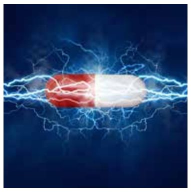


Drug Metabolism

EC-MS has been applied successfully for **fast prediction** and mimicking of oxidative **drug metabolism** (*"in-electro" vs. in-vivo or in- vitro*). The metabolites are formed instantaneously in the electrochemical cell (**biomimetic oxidation**), mimicking the enzymatic biotransformation of the Cytochrome P450 reactions of the liver (Phase I reaction) including adduct formation (Phase II reactions). Compared to conventional in-vivo methods (e.g., rodents, humans) or in-vitro methods (e.g., microsomes), considerable time and cost savings have been published.

Environmental Degradation

EC-MS is used for simulating most major reactions that take place in the environmental degradation process, i.e., **aquatic** (aqueous), **photolytic** (photochemical), **microbial** conversions including adduct formation (phase II). Relevant reactive intermediates useful in the understanding of the transformation (degradation) pathway have been generated by EC – impossible to extract form environmental samples. Again EC-MS is an easy, inexpensive and extremely fast approach to get a first insight into the degradation process of **persistent organic pollutants** (POP's).



Drug Stability

Forced degradation studies are important to obtain information about potential degradation products and their pathways. Oxidative reactions are the most commonly observed degradation pathways for pharmaceuticals. EC as **"green"** and **rapid oxidative stress test** to study the degradation of API's or the influence of excipients has been used successfully, making the use of harsh and toxic oxidizing regents (peroxide, radical initiators) obsolete. Furthermore the EC approach is tuneable, selective and can be scaled up for fast synthesis of mg quantities of degradants.

Electrochemical Synthesis

In most areas of drug discovery & development and for degradation studies of pharmaceuticals/ xenobiotics in environment, there is a need for **reference materials** (i.e., metabolites, degradants, etc.). Scale-up to mg quantities is required for structural identification of these products by MS and NMR, and for subsequent toxicology studies. Conventional strategies such as wet chemistry or enzymatic approaches are time consuming, cumbersome, expensive and often unsuccessful. Electrochemical synthesis is a purely instrumental technique capable of **rapid synthesis in less than 1 hour**.

Introduction

In this document you will find a large collection of references from peer-reviewed scientific journals, using the Antec Scientific ROXY Electrochemistry (EC) system and/or reactor cells. The literature references are grouped per field of application: drug metabolism, drug stability, environmental degradation, electrochemical synthesis, disulfide bond reduction in proteins, etc. For every literature reference the type of electrochemical flow/reactor cell, working electrode (WE), mode of operation oxidative (OX) or reductive (RED) are specified for your convenience. DOI links for easy access to the corresponding articles are available in the '#' column. Some of the publications are open access for others a purchase fee might apply. In case the compound in the table is marked with an '*', both phase I and II reactions are reported in the publication.

Note: this collection of references is a snapshot in time (until Q1/2020) and may not contain the latest publications. For latest literature references use: Google Scholar.

Abbreviations:

CC = ChipCell
RC = ReactorCell
µ-PC = µ-PrepCell (1.0, 2.0 or SS)
SC = SynthesisCell
 # = column with DOI literature link
** = both phase I and II reactions*
OX = Oxidative Mode
RED = Reductive Mode
WE = Working electrode
GC = Glassy Carbon
BDD = Boron Doped Diamond (Magic Diamond)
Ti = Titanium
Pt = Platinum
Au = Gold
Ag = Silver
Cu = Copper

Electrochemistry-MS Reference List

Drug/Xenobiotic Metabolism

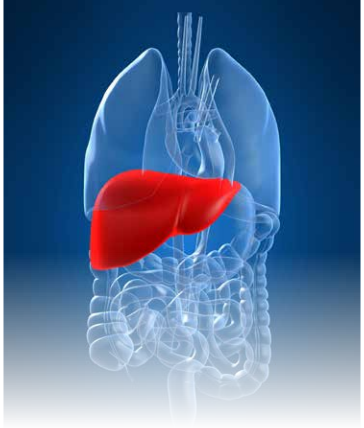


Table 1. Drug / Xenobiotic Metabolism

#	Compound(s)	Reference	Reactor	WE	Mode
2009-01	Tetrazepam	Metabolic studies of tetrazepam based on electrochemical simulation in comparison to in vivo and in vitro methods, A. Baumann, Uwe Karst et al., J. of Chrom. A, 2009, 1216, 3192-3198	RC	GC, Pt, Au	OX
2010-02	Triclocarban	Electrochemistry-Mass Spectrometry Unveils the Formation of Reactive Triclocarban Metabolites, A. Baumann, Uwe Karst et al., Drug Metabolism and Disposition, 2010, 38 (12), 2130-2138	RC	BDD	OX
2011-02	Verapamil	Investigation of the biotransformation pathway of verapamil using electrochemistry/liquid chromatography/mass spectrometry - A comparative study with liver cell microsomes, J. of Chrom. A, 2011, 1218(51), 9210-9220	RC	Pt, Au, Ag, Cu, GC, BDD	OX
2011-04	SB-203580-Iodo (SB-I)	High temperature liquid chromatography hyphenated with ESI-MS and ICP-MS detection for the structural characterization and quantification of halogen containing drug metabolites, J. S. B. de Vlieger, W. M.A. Niessen et al., Analytica Chimica Acta, 2011, 698, 69-76	RC	BDD	OX
2011-05	[18F]isatin	Metabolite Identification of a Radiotracer by Electrochemistry Coupled to Liquid Chromatography with Mass Spectrometric and Radioactivity Detection, A. Baumann, Uwe Karst et al., Anal. Chem., 2011, 83(13), 5415-5421	RC	Au	OX
2012-02	Acetaminophen*	Formation and characterization of covalent guanosine adducts with electrochemistry—liquid chromatography-mass spectrometry, S. Plattner, H. Oberacher et al., J. of Chrom. B, 2012,883-884,198-204	RC	BDD	OX
2012-04	p-phenylenediamine*	Electrochemistry/liquid chromatography/mass spectrometry to demonstrate irreversible binding of the skin allergen p-phenylenediamine to proteins, Rapid communications in mass spectrometry, 2012, 26(12), 1415-1425	RC	BDD	OX
2012-05	Acetaminophen*	Combination of Electrochemistry and Nuclear Magnetic Resonance Spectroscopy for Metabolism Studies, S. Jahn, U. Karst et al., Anal. Chem., 2012, 84(20), 8777-8782	RC	GC	OX
2012-06	p-phenylenediamine*	Electrochemistry/mass spectrometry as a tool in the investigation of the potent skin sensitizer p-phenylenediamine and its reactivity toward nucleophiles, S. Jahn, U. Karst et al., Rapid communications in mass spectrometry, 2012, 26(12), 1453-1464	RC	BDD	OX
2012-07	Galantamine, Lycorine	Metabolic studies of the Amaryllidaceous alkaloids galantamine and lycorine based on electrochemical simulation in addition to in vivo and in vitro models, S. Jahn, U. Karst et al., Analytica Chimica Acta, 2012, 756, 60-72	RC	BDD	OX
2012-08	Diclofenac*	Simulation of the oxidative metabolism of diclofenac by electrochemistry/(liquid chromatography/)mass spectrometry, H. Faber, U. Karst et al., Analytical and Bioanalytical Chemistry, 2012, 403(2), 345-354	RC	BDD	OX
2012-12	Gd-based MRI contrast agents	Identification and quantification of potential metabolites of Gd-based contrast agents by electrochemistry/separations/mass spectrometry, L. Telgmann, U. Karst et al., J. of Chrom. A, 2012, 1240, 147-155	RC	BDD	OX
2012-13	Aniline*	Electrochemical oxidation and protein adduct formation of aniline: a liquid chromatography/mass spectrometry study, D. Melles, U. Karst et al., Analytical and Bioanalytical Chemistry, 2012, 403, 377-384	RC	BDD	OX
2012-14	BIRB796, TAK715, SB203580, DMPIP	On-line electrochemistry-bioaffinity screening with parallel HR-LC-MS for the generation and characterization of modified p38α kinase inhibitors, D. Falck, W. M. A. Niessen et al., Analytical and Bioanalytical Chemistry, 2012, 403, 367-375	RC	GC	OX

Drug/Xenobiotic Metabolism

#	Compound(s)	Reference	Reactor	WE	Mode
2012-15	Mitoxantrone	Improved Conversion Rates in Drug Screening Applications Using Miniaturized Electrochemical Cells with Frit Channels, M. Odijk, A. van den Berg et al., Anal. Chem., 2012, 84(21), 9176-9183	CC	Pt	OX
2012-17	Flunitrazepam (Rohypnol), clona-zepam, chlorpromazine	Investigation of some biologically relevant redox reactions using electrochemical mass spectrometry interfaced by desorption electrospray ionization, M. Lu, C. Wolff, W. Cui, H. Chen, Analytical and Bioanalytical Chemistry, 2012, 403(2), 355-365	RC	BDD	RED, OX
2013-02	BIRB796	EC-SPE-stripline-NMR analysis of reactive products: a feasibility study, D. Falck, W. M. A. Niessen et al., Analytical and Bioanalytical Chemistry, 2013, 405(21), 6711-6720	µ-PC1.0	GC	OX
2013-06	Melarsoprol	Investigation of the biotransformation of melarsoprol by electrochemistry coupled to complementary LC/ESI-MS and LC/ICP-MS analysis, A. Baumann, U. Karst et al., Analytical and Bioanalytical Chemistry, 2013, 405(15), 5249-5258	RC	BDD	OX
2013-08	Selenoxanthene	Simultaneous electrochemical oxidation/ionization of a selenoxanthene revealed by on-line electrospray-high resolution mass spectrometry, H. Simon, U. Karst et al., Electrochimica Acta, 2013, 111, 324-331	RC	BDD	OX
2013-09	Rycal S107, PPARd-agonist GW1516	Using electrochemistry for metabolite simulation and synthesis in preventive doping research: application to the Rycal S107 and the PPARδ-agonist GW1516, S. Jahn, U. Karst et al., Anal. Methods, 2013, 5, 1214-1224	RC	BDD	OX
2013-10	Simvastatin, Lovastatin	Generation of statin drug metabolites through electrochemical and enzymatic oxidations, Smriti Khera, Na Hu, Analytical and Bioanalytical Chemistry, 2013, 405(18), 6009-6018	RC, µ-PC1.0	BDD, GC	OX
2013-11	Eugenol, Isoeugenol*	In chemico evaluation of skin metabolism: Investigation of eugenol and isoeugenol by electrochemistry coupled to liquid chromatography and mass spectrometry, D. Melles, U. Karst et al., J. of Chrom. B, 2013, 913, 106-112	RC	BDD	OX
2013-12	Cimetidine*	Influence of cimetidine and its metabolites on Cisplatin—Investigation of adduct formation by means of electrochemistry/liquid chromatography/ electrospray mass spectrometry, C. Brauckmann, U. Karst et al., J. of Chrom. A, 2013, 1279, 49-57	RC	BDD	OX
2014-03	Harmane	Nonaqueous capillary electrophoresis as separation technique to support metabolism studies by means of electrochemistry and mass spectrometry, Jörg Roscher,U. Karst et al., Electrophoresis, 2014, 35(16), 2386-2391	µ-PC1.0	BBD	OX
2014-07	Methamphetamine, dextromethorphan, benzydamine	Determination of psychostimulants and their metabolites by electrochemistry linked on-line to flowing atmospheric pressure afterglow mass spectrometry, M. Smoluch, J. Silberring et al., Analyst, 2014, 139, 4350-4355	µ-PC1.0	BDD, GC	OX
2014-08	Cocaine	Electrochemical simulation of cocaine metabolism—a step toward predictive toxicology for drugs of abuse, P. Mielczarek, J. Silberring et al., Eur J Mass Spectrom,2014, 20(4), 279-285	RC	BDD	OX
2014-10	Tryptamines, cannabinoids, Cathinones	Electrochemical simulation of phase I metabolism for 21 drugs using four different working electrodes in an automated screening setup with MS detection, A. Just Pedersen, W. Weinmann et al., Bioanalysis, 2014, 6(19), 2607-2621	RC	GC, BDD, Au, Pt	OX
2014-13	flavonoids, phenolic acids, anthocyanins	Characterization of Phenolic Compounds and Antioxidant Activity of Solanum scabrum and Solanum burbankii Berries, J. Oszmianski, J. Kolniak-Ostek, A. Wojdło, J. Agric. Food Chem., 2014, 62, 1512–1519	RC	GC	OX
2015-02	Nitrosothiol, nitrosylated insulin B , carbamazepine	Online Investigation of Aqueous-Phase Electrochemical Reactions by Desorption Electrospray Ionization Mass Spectrometry, M. Lu, H. D. Dewald, Hao Chen et al., Journal of The American Society for Mass Spectrometry, 2015, 26(10), 1676-1685	RC, µ-PC1.0	Au, GC	RED, OX
2015-03	LGD-4033	Characterization of a non-approved selective androgen receptor modulator drug candidate sold via the Internet and identification of in vitro generated phase-I metabolites for human sports drug testing, M. Thevis, U. Karst et al., Rapid communication in mass spectrometry, 2015, 29, 11, 991-999	RC, µ-PC1.0	BDD	OX

#	Compound(s)	Reference	Reactor	WE	Mode
2015-09	Colchicine	Mechanistic study of colchicine's reduction behavior, E. Bodoki, L. Vlase, R. Săndulescu, Electrochemistry Communications, 2015, 56, 51-55	RC	BDD	RED
2015-10	Selegiline	Electrochemical generation of selegiline metabolites coupled to mass spectrometry, P. Mielczarek, J. Silberring et al., J. of Chrom. A, 2015, 1389, 96-103	RC	GC, BDD	OX
2015-11	Colchicine	Mechanistic study of colchicine's electrochemical oxidation, E. Bodoki, R. Chira, V. Zaharia, R. Săndulescu, Electrochimica Acta, 2015, 178, 624-630	RC	BDD	OX
2015-12	Lidocaine	Optimization of reaction parameters for the electrochemical oxidation of lidocaine with a Design of Experiments approach, T. Gul, R. Bischoff, H. P. Permentier, Electrochimica Acta, 2015, 171, 23-28		Au, GC	OX
2015-14	Amodiaquine, chlorpromazine, clozapine	Mass Spectrometric Detection of Short-Lived Drug Metabolites Generated in an Electrochemical Microfluidic Chip, F. T. G. van den Brink, M. Odijk, U. Karst, A. van den Berg et al., Anal. Chem., 2015, 87(3), 1527-1535	SC	Pt	OX
2016-06	Chrysin, flavonol, kaempferol, morin, quercetin, myricetin	Oxidation of Flavonols in an Electrochemical Flow Cell Coupled Online with ESI-MS, S. Kummer, W. Ruth, U. Kragl, Electroanalysis, 2016, 28(5), 990-997	RC	GC	OX
2016-07	3-Methylcatechol*	Electrochemical Initiated C-N Coupling of 3-Methylcatechol and n-Hexylamine in a Flow Cell Monitored with ESI-MS, S. Kummer, W. Ruth, U. Kragl, Electroanalysis, 2016, 28(9), 1992-1999	RC	GC	OX
2016-08	amoxicillin, cefotaxime, fluconazole, linezolid, metronidazole and moxifloxacin	Electrochemistry-mass spectrometry for in-vitro determination of selected chemotherapeutics and their electrochemical products in comparison to in-vivo approach, M. Szultka-Mlynska, B. Buszewski, Talanta,2016, 160, 694-703	RC	GC, BDD	OX
2016-09	Alternariol, Alternariol methyl ether	Electrochemical simulation of metabolic reactions of the secondary fungal metabolites alternariol and alternariol methyl ether, H. Simon, U. Karst et al., Analytical and Bioanalytical Chemistry, 2016, 408, 2471-2483	RC	BDD	OX
2016-10	Epinephrine	Epinephrine sensing at nanostructured Au electrode and determination its oxidative metabolism, E. Wierzbicka, B. Buszewski et al., Sensors and Actuators B: Chemical, 2016, 237, 206-215	RC	Au	OX
2016-11	Homologous series of fluorinated spirocyclic s1 receptor ligands	Comparison of in Silico, Electrochemical, in Vitro and in Vivo Metabolism of a Homologous Series of (Radio)fluorinated σ1 Receptor Ligands Designed for Positron Emission Tomography, C. Wiese, U. Karst, B. Wünsch et al., Chem med chem, 2016, 11(21), 2445-2458	RC	BDD	OX
2016-12	KAE609 (Cipargamin)	KAE609 (Cipargamin), a New Spiroindolone Agent for the Treatment of Malaria: Evaluation of the Absorption, Distribution, Metabolism, and Excretion of a Single Oral 300-mg Dose of [14C] KAE609 in Healthy Male Subjects, S. W. Huskey, D. S. Stein et al., Drug metabolism and disposition, 2016, 44, 672-682	SC	BBD	OX
2016-14	NAC, GSH and cysteine*	Comparative study of the oxidation behavior of sulfur-containing amino acids and glutathione by electrochemistry-mass spectrometry in the presence and absence of cisplatin, R. Zabel, G. Weber, Analytical and Bioanalytical Chemistry, 2016, 408(4), 1237-1247	RC	BDD	OX
2016-15	1-hydroxypyrene*	Oxidation and adduct formation of xenobiotics in a microfluidic electrochemical cell with boron doped diamond electrodes and an integrated passive gradient rotation mixer, F. T. G. van den Brink, M. Odijk, U. Karst, A. van den Berg et al., Lab Chip, 2016, 16, 3990-4001	SC	BDD	OX
2017-02	Chicoric acid	Mechanism of Chicoric Acid Electrochemical Oxidation and Identification of Oxidation Products by Liquid Chromatography and Mass Spectrometry, E. F. Newair, R. Abdel-Hamid, P. A. Kilmartin, Electroanalysis, 2017, 29,3,850-860	μ-PC1.0	GC	OX
2017-07	Chlorpyrifos	Electrochemistry coupled online to liquid chromatography-mass spectrometry for fast simulation of biotransformation reactions of the insecticide chlorpyrifos, T. F. Mekonnen, U. Panne, M. Koch, Analytical and Bioanalytical Chemistry, 2017, 409(13), 3359-3368	μ-PC1.0	BDD	OX

#	Compound(s)	Reference	Reactor	WE	Mode
2017-09	Lidocaine	Mechanism of aromatic hydroxylation of lidocaine at a Pt electrode under acidic conditions, T. Gul, R. Bischoff, H. P.Permentier, Analytica Chimica Acta, 2017, 993, 1-21		Pt	OX
2017-11	Roxarsone *	Investigation of the oxidative transformation of roxarsone by electrochemistry coupled to hydrophilic interaction liquid chromatography/mass spectrometry, L. M. Frensemeier, U. Karst et al., Electrochimica Acta, 2017, 224, 636-641	µ-PC1.0	BDD	OX
2017-12	Triapine*	Understanding the metabolism of the anticancer drug Triapine: electrochemical oxidation, microsomal incubation and in vivo analysis using LC-HRMS, K. Pelivan, U. Karst et al., Analyst, 2017, 142, 3165-3176	RC	BDD	OX
2018-01	Z-ligustilide	Preparing the key metabolite of Z-ligustilide in vivo by a specific electro-chemical reaction, F. Duan, H. Xiao et al., J. Anal. At. Spectrom., 2017, 32, 153	µ-PC2.0, SC	GC	OX
2018-03	Fluopyram	Prediction of biotransformation products of the fungicide fluopyram by electrochemistry coupled online to liquid chromatography-mass spectrometry and comparison with in vitro microsomal assays, Tessema F. Mekonnen, U. Panne ,M. Koch, Analytical and Bioanalytical Chemistry, 2018, 410, 2607-2617	µ-PC2.0, SC	BDD	OX
2018-04	Eriodictyol*	Mechanistic Pathways and Identification of the Electrochemically Generated Oxidation Products of Flavonoid Eriodictyol in the Presence of Glutathione, E. F. Newair, F. Garcia et al., Electroanalysis, 2018, 30(8), 1714-1722	µ-PC1.0	GC	OX
2019-05	Imidazoacridinone C-1311	Electrochemical simulation of metabolism for antitumor-active imidazoacridinone C-1311 and in silico prediction of drug metabolic reactions, A. Potęga, Z. Mazerska et al., Journal of Pharmaceutical and Biomedical Analysis, 2019, 169, 269-278	RC	GC	OX
2019-08	Vitamine D (cholecalciferol, ergocalciferol)	Electrochemical Oxidation as a Tool for Generating Vitamin D Metabolites, L. Navarro Suarez, S. Rohn et al., Molecules, 2019, 24,13, 2369	µ-PC1.0	GC, BBD	OX
2019-09	Cyclosporine A, Everlimus, mycophenolic acid, Siroli-mus, Tacrolimus*	Electrochemical oxidation of selected immunosuppressants and identification of their oxidation products by means of liquid chromatography and tandem mass spectrometry, M. Szultka-Mlynska, B. Buszewski, Journal of Pharmaceutical and Biomedical Analysis, 2019, 176,1 12799	RC	BDD (GC, Pt, Au)	OX
2019-11	Azo dyes: Sudan I - IV, Para RED	Electrochemical reduction of azo dyes mimicking their biotransformation to more toxic products, K. Pietruk, M. Piątkowska, M. Olejnik, J .Vet. Res., 2019, 63, 433-438	RC	GC	RED
2020-01	Salvianolic acid C, Ros-marinic acid, lithospermic acid, protocatechuic alde-hyde, salvianolic acid B*	Oxidative metabolism of typical phenolic compounds of Danshen by electrochemistry coupled to quadrupole time-of-flight tandem mass spectrometry, J.Yang, J. Cao et al., Food Chemistry, 2020, online	RC	GC	OX
2020-02	Triazoloacridinone C-1305	Electrochemical and in silico approaches for liver metabolic oxidation of antitumor-active triazoloacridinone C-1305, A. Potega, Z. Mazerska et al., Journal of Pharmaceutical analysis, 2020, online	RC	GC	OX
2020-06	Metoprolol	Fast Online Separation and Identification of Electrochemically Generated Isomeric Oxidation Products by Trapped Ion Mobility-Mass Spectrometry, J. Fangmeyer, U. Karst et al., Anal. Chem. , 2020, 92(1), 1205-1210	µ-PC2.0	BDD	OX
2018-05	Sinapinic acid, Ferulic acid, Chlorogenic acid, Caffeic acid*	Analysis of Protein-Phenolic Compound Modifications Using Electrochemistry Coupled to Mass Spectrometry, C. Kallinich, S. Schefer, S. Rohn, J. of Separation Science, 2018, 41(13), 2799-2807	µ-PC1.0	BDD	OX
2018-07	Metoprolol, Propranolol, Propafenone, Mexiletine, Oxprenolol, Pirbuterol, Pindolol, Cicloprolol, Ace-butolol, Atenolol*	Structural characterization of electrochemically and in vivogenerated potential metabolites of selected cardiovascular drugs by EC-UHPLC/ESI-MS using an experimental design approach, M. Szultka-Młyńska, B. Buszewski et al., Molecules, 2018, 23(2), 246	RC	GC, Pt, Au, BDD	OX
2018-08	Combretastatin A4	Untargeted screening of phase I metabolism of combretastatin A4 by multi-tool analysis, K. Jarocha, B. Bojko et al., Talanta, 2018, 176, 262-276	RC	Au, GC, BDD	OX

#	Compound(s)	Reference	Reactor	WE	Mode
2018-09	Rivaroxaban, Aliskiren, Prasugrel	Electrochemical simulation of three novel cardiovascular drugs phase I metabolism and development of a new method for determination of them by liquid chromatography coupled with tandem mass spectrometry, M. Szultka-Młyńska, B. Buszewski et al., Talanta, 2018, 182, 22-31	RC	GC, Pt, Au, BDD	OX
2018-12	cholic acid, chenodeoxy-cholic acid	Electrochemical Oxidation of Primary Bile Acids: A Tool for Simulating Their Oxidative Metabolism, L. N. Suarez, L. Brückner, S. Rohn, Int. J. Mol. Sci., 2018, 19, 9, 2491	u-PC1.0, SC	BDD	OX
2018-15	Chlorpyrifos	Investigation of Chlorpyrifos and Its Transformation Products in Fruits and Spices by Combining Electrochemistry and Liquid Chromatography Coupled to Tandem Mass Spectrometry, T. F. Mekonnen, M. Koch et al., Food Analytical Methods,2018, 11, 10,2657-2665	SC	BDD	OX
2018-16	OxPt(Succ)(Oac), OXPt(Succ)2, CisPt(Succ)(OAc), Satraplatin	Structure elucidation and quantification of the reduction products of anticancer Pt(IV) prodrugs by electrochemistry/mass spectrometry (EC-MS), L. M. Frensemeier, U. Karst et al., J. of Chrom. B, 2018, 1093, 100-112	µ-PC2.0	Ti	RED
2019-01	Auranofin, Aubipyc	The electrochemical profiles of Auranofin and Aubipyc, two representative medicinal gold compounds: A comparative study, M. Kupieca, K. Pawlak et al., Analyst, 2018, 143, 1997-2001	RC	BDD	OX, RED
2019-02	Chardonnay (white wine)	Electrochemical triggering of the Chardonnay wine metabolome, C. Roullier-Gallab, P. Schmitt-Kopplin, Food Chemistry, 2019, 286, 2019, 64-70	µ-PC1.0	BDD	OX
2019-03	2-hydroxyacridinone*	Phase I and phase II metabolism simulation of antitumor-active 2-hydroxyacridinone with electrochemistry coupled on-line with mass spectrometry, A. Potęga, Z. Mazerska et al., Journal of Inorganic Biochemistry, 2019, 198, 110714	RC	GC	OX

Table 2. Drug Stability

#	Compound(s)	Reference	Reactor	WE	Mode
2014-04	Fesoterodine	Rapid Synthesis of Pharmaceutical Oxidation Products Using Electrochemistry: A Systematic Study of N-Dealkylation Reactions of Fesoterodine Using a Commercially Available Synthesis Cell, S. Torres, M. R. Taylor et al., Org. Process Res. Dev., 2015, 19(11), 1596-1603	SC	RGC	OX
2015-04	Ezlopitant	The application of electrochemistry to pharmaceutical stability testing - Comparison with in silico prediction and chemical forced degradation approaches, S. Torres, M. R. Taylor et al., Journal of Pharmaceutical and Biomedical Analysis, 2015, 115, 487-501	RC, µ-PC1.0	GC	OX
2016-04	Ezlopitant	Electrochemical oxidation coupled with liquid chromatography and mass spectrometry to study the oxidative stability of active pharmaceutical ingredients in solution: A comparison of off-line and on-line approaches, S. Torres, M. R. Taylor et al., Journal of Pharmaceutical and Biomedical Analysis, 2016, 131, 71-79	µ-PC1.0	GC	OX

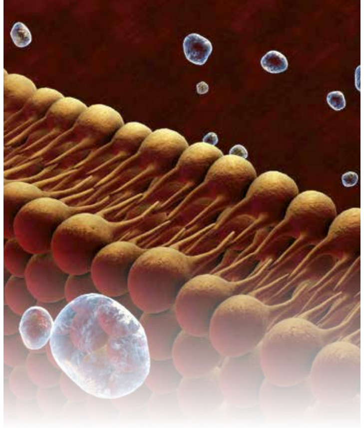


Table 3. Lipids Oxidation

#	Compound(s)	Reference	Reactor	WE	Mode
2016-02	Cholesterol	Electrochemical oxidation of cholesterol: An easy way to generate numerous oxysterols in short reaction times, D. Weber, Z. Ni, D. Vetter, R. Hoffmann, M. Fedorova, European Journal of Lipid Science and Technology, 2016, 118(2), 325-331	µ-PC2.0	BDD	OX
2018-03	POPE, PLPE, PAPE	Electrochemical oxidation of phosphatidylethanolamines studied by mass spectrometry, S. Colombo, G. Coliva, A. Kraj, J-P. Chervet, M. Fedorova et al., Journal of mass spectrometry, 2018, 53(3), 223-233	µ-PC2.0	BDD	OX
2020-08	Sphingomyelins	Sphingomyelins prevent propagation of lipid peroxidation - LC-MS/MS evaluation of inhibition mechanisms, G. Coliva, M. Lange, S. Colombo, J.P. Chervet, R. Domingues, M. Fedorova, Molecules, special issue Mass Spectrometry Based Lipidomics, Molecules, 2020, 25(8), 1925	µ-PC2.0	BDD	OX

Table 4. DNA/RNA Damage

#	Compound(s)	Reference	Reactor	WE	Mode
2010-01	DNA/RNA nucleotides	On-Line Electrochemistry/Electrospray Ionization Mass Spectrometry (EC/ESI-MS) for the Generation and Identification of Nucleotide Oxidation Products, A. Baumann , W. Lohmann, S. Jahn, U. Karst, Electroanalysis, 2010, 22(3), 286-292	RC	BDD	OX
2010-03	DNA nucleotides	Electrochemical simulation of oxidation processes involving nucleic acids monitored with electrospray ionization-mass spectrometry, F. Pitterl, J-P. Chervet, H. Oberacher, Analytical and Bioanalytical Chemistry, 2010, 397(3), 1203-1215	RC	BDD	OX

Electrochemical Synthesis

Table 5. Electrochemical Synthesis

#	Compound(s)	Reference	Reactor	WE	Mode
2014-04	Fesoterodine	Rapid Synthesis of Pharmaceutical Oxidation Products Using Electrochemistry: A Systematic Study of N-Dealkylation Reactions of Fesoterodine Using a Commercially Available Synthesis Cell, S. Torres, M. R. Taylor et al., Org. Process Res. Dev., 2015, 19(11), 1596-1603	SC	RGC	OX
2015-06	Carbamazepine	An efficient laboratory workflow for environmental risk assessment of organic chemicals, L. Zhu, S. Küppers et al., Analytical and Bioanalytical Chemistry, 2014, 406(28), 7253-7260	SC	BDD	OX
2016-05	Ciprofloxacin, Norfloxacin, Ofloxacin	Electrochemical oxidation of fluoroquinolone antibiotics: Mechanism, residual antibacterial activity and toxicity change, M-A. Lecours, P. A. Segura et al., Water Research, 2016, 102,5 2-62	SC	BDD	OX
2016-12	KAE609 (Cipargamin)	KAE609 (Cipargamin), a New Spiroindolone Agent for the Treatment of Malaria: Evaluation of the Absorption, Distribution, Metabolism, and Excretion of a Single Oral 300-mg Dose of [14C] KAE609 in Healthy Male Subjects, S. W. Huskey, D. S. Stein et al., Drug metabolism and disposition, 2016, 44, 672-682	SC	BBD	OX
2018-01	Z-ligustilide	Preparing the key metabolite of Z-ligustilide in vivo by a specific electrochemical reaction, F. Duan, H. Xiao et al., J. Anal. At. Spectrom., 2017, 32, 153	SC	GC	OX
2018-03	Fluopyram	Prediction of biotransformation products of the fungicide fluopyram by electrochemistry coupled online to liquid chromatography-mass spectrometry and comparison with in vitro microsomal assays, Tessema F. Mekonnen, U. Panne ,M. Koch, Analytical and Bioanalytical Chemistry, 2018, 410, 2607-2617	SC	BDD	OX
2018-11	Biaryl Ether-Linked Zearalenone Dimer	Synthesis and Structural Identification of a Biaryl Ether-Linked Zearalenone Dimer, J. Keller, L. Hantschke, H. Haase, M. Koch, Molecules, 2018, 23(10), 2624	SC	Pt	OX
2018-12	cholic acid, chenodeoxycholic acid	Electrochemical Oxidation of Primary Bile Acids: A Tool for Simulating Their Oxidative Metabolism, L. N. Suarez, L. Brückner, S. Rohn, Int. J. Mol. Sci., 2018, 19, 9, 2491	SC	BDD	OX
2018-14	Triclosan	Electrochemical simulation of triclosan metabolism and toxicological evaluation, L. Zhu, S. Küppers et al., Science of The Total Environment, 2018, 622, 1193-1201	SC	BDD	OX
2018-15	Chlorpyrifos	Investigation of Chlorpyrifos and Its Transformation Products in Fruits and Spices by Combining Electrochemistry and Liquid Chromatography Coupled to Tandem Mass Spectrometry, T. Fenta Mekonnen, L. Byrne, U. Panne, M. Koch, Food Analytical Methods, 2018, 11(10), 2657-2665	SC	BDD	OX

Electrochemistry-MS Reference List

Environmental Degradation

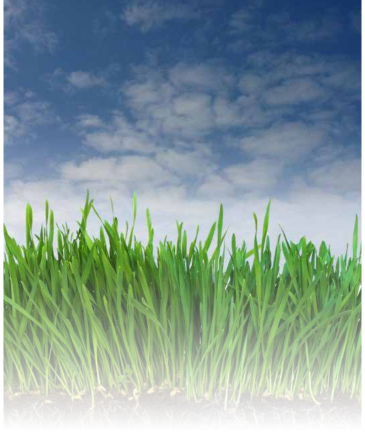


Table 6. Environmental Degradation

#	Compound(s)	Reference	Reactor	WE	Mode
2011-03	Sulfadiazine	Electrochemistry-mass spectrometry for mechanistic studies and simulation of oxidation processes in the environment, Th. Hoffmann, S. Küppers et al., Analytical and Bioanalytical Chemistry, 2011, 399(5), 1859-18681	RC	BDD	OX
2012-10	Methabenzthiazuron, Ethidimuron, Propanil	Bottom-up approach for the reaction of xenobiotics and their metabolites with model substances for natural organic matter by electrochemistry-mass spectrometry (EC-MS), L. Chen, S. Küppers et al. , Chemosphere, 2012, 89(11), 1376-1383	RC	GC, BDD	OX, RED
2013-07	2,4',5-trichlorobiphenyl	Online electro-Fenton-mass spectrometry reveals 2,4' ,5-trichlorobiphenyl oxidation products and binding to organic matter, L. Chen, S. Küppers et al. , Environmental Chemistry Letters, 2014, 12(2), 329-334	RC	BDD	OX
2014-02	Diclofenac, Metoprolol	Liquid chromatography/mass spectrometry to study oxidative degradation of environmentally relevant pharmaceuticals by electrochemistry and ozonation, H. Faber, U. Karst et al., Journal of Chromatography A, 2014,1 343, 152-159	µ-PC1.0	BBD	OX
2014-11	3-trifluoromethyl-4-nitrophenol, Niclosamide, Nilutamide	Phase I and phase II reductive metabolism simulation of nitro aromatic xenobiotics with electrochemistry coupled with high resolution mass spectrometry, U. Bussy, W. Li et al. , Chemosphere, 2015, 131, 34-40	RC	BDD	OX
2015-06	Carbamazepine	An efficient laboratory workflow for environmental risk assessment of organic chemicals, L. Zhu, S. Küppers et al., Analytical and Bioanalytical Chemistry, 2014, 406(28), 7253-7260	RC	BDD	OX
2015-07	Carbamazepine	Electrochemistry Combined with LC-HRMS: Elucidating Transformation Products of the Recalcitrant Pharmaceutical Compound Carbamazepine Generated by the White-Rot Fungus Pleurotus ostreatus, E. Jahangiri, B. Seiwert, T. Reemtsma, D. Schlosser, Environ. Sci. Technol., 2015, 49(20), 12342-12350	RC	BDD	OX
2016-05	Ciprofloxacin, Norfloxacin, Ofloxacin	Electrochemical oxidation of fluoroquinolone antibiotics: Mechanism, residual antibacterial activity and toxicity change, M-A. Lecours, P. A. Segura et al., Water Research, 2016, 102,5 2-62	RC, SC	BDD	OX
2016-13	Carbamazepine	Reductive transformation of carbamazepine by abiotic and biotic processes, A. König, T.n Reemtsma, M. Jekel et al., Water Research, 2016, 101, 272-280	µ-PC1.0	GC, BDD	RED
2017-06	Triclosan	Laccase- and electrochemically mediated conversion of triclosan: Metabolite formation and influence on antibacterial activity, E. Jahangiri, B. Seiwert, T. Reemtsma, D. Schlosser , Chemosphere, 2017, 168, 549-558	RC	BDD	OX
2018-02	Trimethoprim	Electrochemistry-High Resolution Mass Spectrometry to Study Oxidation Products of Trimethoprim, M-A. Lecours, P. A. SeguraEnvironments,2018 5,1,18	µ-PC1.0	BDD	OX
2018-10	Oxytetracycline	Transformation of oxytetracycline by redox-active Fe(III)- and Mn(IV)-containing minerals: Processes and mechanisms, M. Karpova, Thorsten Reemtsma, B. Chefetz et al., Water Research, 2018, 145, 136-145	RC	BDD	OX
2018-14	Triclosan	Electrochemical simulation of triclosan metabolism and toxicological evaluation, L. Zhu, S. Küppers et al., Science of The Total Environment, 2018, 622, 1193-1201	RC, SC	BDD	OX
2019-06	Monensin	Prediction of Transformation Products of Monensin by Electrochemistry Compared to Microsomal Assay and Hydrolysis, L. Kotthoff, M. Koch et al., Molecules, 2019, 24, 2732	µ-PC1.0	GC, BBD	OX

Environmental Degradation

#	Compound(s)	Reference	Reactor	WE	Mode
2019-12	Difenoconazole	Electrochemical Oxidation of Difenoconazole in Solutions: LC/MS Identification of Reaction Products, T. I. Pushkareva, I. G. Zenkevich, Moscow Univ. Chem. Bull., 2019, 74, 127-133	RC	BDD	OX
2020-03	moxidectin	Structural annotation of electro- and photochemically generated transformation products of moxidectin using high-resolution mass spectrometry, L. Kotthoff, M. Koch et al., Analytical and Bioanalytical Chemistry, 2020, online	µ-PC2.0	BDD	OX

Electrochemistry-MS Reference List

Disulfide Bond Reduction in Proteins/Peptides

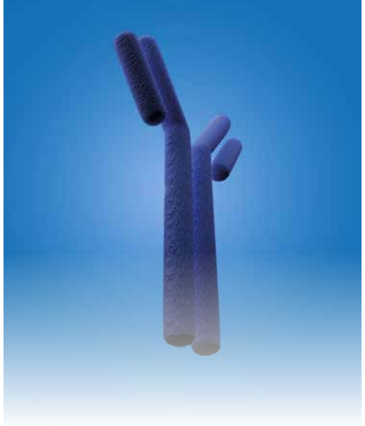


Table 7. Disulfide bond Reduction in Proteins & Peptides

#	Compound(s)	Reference	Reactor	WE	Mode
2009-02	GSSH, NRCSQSCWN peptide, Bovine Insuline, b-lactoglobulin	Online Coupling of Electrochemical Reactions with Liquid Sample Desorption Electrospray Ionization-Mass Spectrometry, J. Li, H. D. Dewald, and H. Chen, Analytical Chemistry, 2009, 81(23), 9716— 9722		Au-amal-gam	RED
2011-01	Somatostatin	Coupling of liquid chromatography with mass spectrometry by desorption electrospray ionization (DESI), Y. Zhang, Hao Chen et al., Chem. Commun., 2011, 47, 4171-4173	μ-PC1.0	BDD	RED
2011-06	[arg8]-Conopressin G, Somastatin, Insulin	Online mass spectrometric analysis of proteins/peptides following electrolytic cleavage of disulfide bonds, Y. Zhang, Hao Chen et al., J. Proteome Res., 2011, 10(3), 1293-1304	μ-PC1.0	Au-amal-gam	RED
2012-01	β-lactoglobulin A	Electrochemistry-Assisted Top-Down Characterization of Disulfide-Containing Proteins, Y. Zhang, Hao Chen et al., Anal. Chem, 2012, 84(8), 3838-3842	μ-PC1.0	BDD	RED
2013-01	Oxytocin, Hepcidin	On-Line Electrochemical Reduction of Disulfide Bonds: Improved FTICR-CID and -ETD Coverage of Oxytocin and Hepcidin, S. Nicolardi, A. Kraj, J-P. Chervet, A. M. Deelder, Y. E. M. van der Burgt et al., Journal of The American Society for Mass Spectrometry, 2013, 24(12), 1980-1987	μ-PC1.0	Ti	RED
2013-03	Bovine Insulin	Integration of online digestion and electrolytic reduction with mass spec-trometry for rapid disulfide-containing protein structural analysis, Q. Zheng, H. Zhang, H. Chen, International Journal of Mass Spectrometry, 2013,3 53,8 4-92	μ-PC1.0	BBD	RED
2013-05	Bovine Insulin	A novel electrochemical method for efficient reduction of disulfide bonds in peptides and proteins prior to MS detection, A. Kraj, H-J. Brouwer, N. Reinhoud, J-P. Chervet, Analytical and Bioanalytical Chemistry, 2013, 405(29), 9311-9320	μ-PC1.0	Ti	RED
2014-01	Insulin, uPAR	Electrochemical Reduction of Disulfide-Containing Proteins for Hydrogen/Deuterium Exchange Monitored by Mass Spectrometry, S. Mysling, R. Salbo, M. Ploug, T. J. D. Jørgensen, Anal. Chem, 2014, 86(1), 340-345	μ-PC1.0-HP	Ti	red
2014-05	HCK3FWW, Bovine Insulin, Tryptic digest of cross-linked ubiquitin	Cross-Linking Electrochemical Mass Spectrometry for Probing Protein Three-Dimensional Structures, Q. Zheng, H. Zhang, H. Chen et al., Anal. Chem., 2014, 86(18), 8983-8991	μ-PC1.0	BBD	RED
2014-09	Intact IgG1 mAb	Structural Analysis of an Intact Monoclonal Antibody by Online Electrochemical Reduction of Disulfide Bonds and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, S. Nicolardi, A. M. Deelder, Y. E. M. van der Burgt, Anal. Chem, 2014, 86(11,) 5376-5382	μ-PC1.0	Ti	RED
2015-05	Somatostatin, Bovine Insulin, myoglobin, and a-lactalbumin	Integration of Electrochemistry with Ultra-Performance Liquid Chromatography/Mass Spectrometry, Y. Cai, Q. Zheng, H. Chen et al., European Journal of Mass Spectrometry, 2015, 21(3), 341-351	μ-PC1.0	BDD	RED
2016-03	dithiobis[succinimidyl pro-pionate] (DSP-d0 and DSP-d8), SLIGKV-NH2 peptide	Probing Protein 3D Structures and Conformational Changes Using Electrochemistry-Assisted Isotope Labeling Cross-Linking Mass Spectrometry, Q. Zheng, H. Zhang, H. Chen et al., Journal of The American Society for Mass Spectrometry, 2016, 27(5), 864-875	μ-PC1.0	BDD	RED
2016-17	Ribonuclease B, ß-lacto-globulin	In-Depth Characterization of Protein Disulfide Bonds by Online Liquid Chromatography-Electrochemistry-Mass Spectrometry, L. Switzar, S. Nicolardi, Julie, Y. E. M. van der Burgt et al., J. Am. Soc. Mass Spectrom., 2016, 27, 50-58	μ-PC1.0	Ti	RED

Disulfide Bond Reduction in Proteins/Peptides

#	Compound(s)	Reference	Reactor	WE	Mode
2012-17	Apamin, Endothelin	Investigation of some biologically relevant redox reactions using electrochemical mass spectrometry interfaced by desorption electrospray ionization, M. Lu, C. Wolff, W. Cui, H. Chen, Analytical and Bioanalytical Chemistry, 2012, 403(2), 355-365	RC	BDD	RED
2015-01	IgG1 (PDB-ID: 1IGY), NGF (PDB-ID: 1BET)	Conformational Analysis of Large and Highly Disulfide-Stabilized Proteins by Integrating Online Electrochemical Reduction into an Optimized H/D Exchange Mass Spectrometry Workflow, E. Trabjerg, R. U. Jakobsen, K. D. Rand et al., Anal. Chem, 2015, 87(1), 78880-78888	µ-PC 1.0-HP	Ti	RED
2016-01	Human Insulin, Lysozyme	Disulfide Linkage Characterization of Disulfide Bond-Containing Proteins and Peptides by Reducing Electrochemistry and Mass Spectrometry, C. N. Cramer, Peter Kresten Nielsen et al, Anal. Chem, 2016, 88(3), 1585-1592	µ-PC 1.0-HP	Ti	RED
2017-03	pro-Nerve growth factor-b	Conformational characterization of nerve growth factor-β reveals that its regulatory pro-part domain stabilizes three loop regions in its mature part, E. Trabjerg, K. D. Rand et al., J. Biol. Chem., 2017, 292(40), 16665-16676	µ-PC 1.0-HP	Ti	RED
2017-04	Oxidized Glutathion (GSSG), Oxytocin, Bovin insulin	Dual reductive/oxidative electrochemistry/liquid chromatography/mass spectrometry: Towards peptide and protein modification, separation and identification, L. Büter, L. M. Frensemeier, U. Karst et al., Journal of Chromatography A, 2017, 1479, 153-160	RC (OX, label-ling), µ-PC1.0 (RED)	BDD (OX), Ti (RED)	OX, RED
2020-07	Bovine Insuline, Vascular Endothelial Growth Factor (VEGF)	Hydrogen/Deuterium exchange mass spectrometry with improved electrochemical reduction enables comprehensive epitope mapping of a therapeutic antibody to the cysteine-knot containing Vascular Endothelial Growth Factor, G.Comamala, C. Wagner, P. Sanz, R. U Jakobsen; M. Koenig; H.J. Brouwer, K. D Rand, Analytica Chimica Acta, 2020, 1115, 41-51	µ-PC-SS	Ti	RED

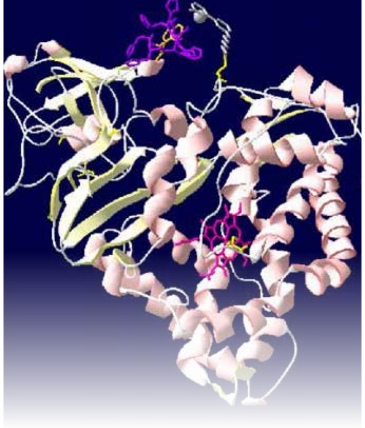


Table 8. Peptide Bond Cleavage

#	Compound(s)	Reference	Reactor	WE	Mode
2010-06	Tyr and Trp-containing tripeptides (LYL, GYG, EYE, KYK, LWL, GWG, EWE, KWK)	Electrochemical Oxidation and Cleavage of Tyrosine- and Tryptophan-Containing Tripeptides, J. Roeser, H. P. Permentier, A. P. Bruins, R. Bischoff, Anal. Chem, 2010, 82, 18, 7556-7565		porous graphite	OX
2012-16	GGYR, SAWGSWS	Peptide cleavage and oxidation using ROXY EC system with on-line mass spectrometry detection, P. Mielczarek, H. Raoof, J. Silberring, Biomacromolecular Mass spectrometry, 2011, 2, 4, 304-310	RC	BDD	OX
2017-10	LYL, Lysozyme	Specific Affinity Enrichment of Electrochemically Cleaved Peptides Based on Cu(II)-Mediated Spirolactone Tagging, T. Zhang, M. P. de Vries, H. P. Permentier, Rainer Bischoff, Anal. Chem.,2017, 89(13),7123-7129	u-PC1.0	BDD	OX

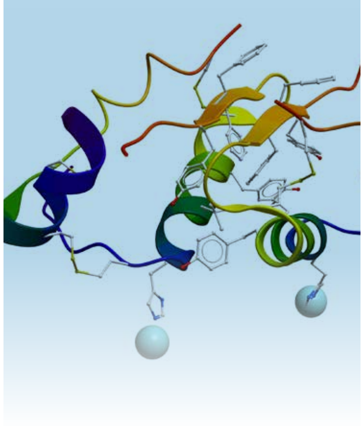


Table 9. Peptide/Protein Labelling

#	Compound(s)	Reference	Reactor	WE	Mode
2015-08	Glutathion, β-lactoglobulin A, Human serum albumin, Bovine serum albumin, Hemoglobin, Human carbonic anhydrase I	Differential Protein Labeling Based on Electrochemically Generated Reactive Intermediates, L. Büter, H. Faber, T. Wigger, M. Vogel, U. Karst, Anal. Chem., 2015, 87(19), 9931-9938	RC	BDD	OX
2017-10	LYL, Lysozyme	Specific Affinity Enrichment of Electrochemically Cleaved Peptides Based on Cu(II)-Mediated Spirolactone Tagging, T. Zhang, M. P. de Vries, H. P. Permentier, Rainer Bischoff, Anal. Chem.,2017, 89(13),7123–7129	u-PC1.0	BDD	OX

Quantification using EC-MS

Table 10. Quantification using EC-MS

#	Compound(s)	Reference	Reactor	WE	Mode
2019-04	Dopamine, Epinephrine, GSSG, uric acid	A New Quantification Method Using Electrochemical Mass Spectrometry, Chang Xu, Qiuling Zheng, Pengyi Zhao, Joseph Paterson, Hao Chen, Journal of The American Society for Mass Spectrometry, 2019, 30, 4, 685-693	RC	BDD	OX, RED
2019-10	Dopamine (DA), Serotinin (5-HT), Norepinephrine (NA)	Improvements for absolute quantitation using electrochemical mass spectrometry, P. Zhao, Y. Guo, H. D. Dewald, H. Chen, Int. J. Mass Spectrom., 2019, 443, 41-45		GC	OX
2019-07	Peptides containing one tyrosine residue: GGYR, DRVY, oxytocin, [Arg]-vasotocin, phosphorylated UOM9	Absolute Quantitation of Oxidizable Peptides by Coulometric Mass Spectrometry, P. Zhao, R. N. Zare, H. Chen, Am. Soc. Mass Spectrom. , 2019, 30(11), 2398-2407	RC	BDD	OX
2020-09	β-casein, apomyoglobin, circadian clock protein KaiB	Absolute Quantitation of Proteins by Coulometric Mass, Spectrometry, P. Zhao, H. Chen et al., Anal. Chem., 2020, publication date May 5th 2020 online		GC	OX

Table 11. Others

#	Compound(s)	Reference	Reactor	WE	Mode
2012-03	Imipramine, Tamoxifen, Reserpine, Amodiaquine, Clomipramine, Morphine, Nalbuphine, Sulfathiourea, Olanzapine, Reproterol, Ticlopidine, Practolol, Acetaminophen, Suolfamethoxazol, Diclofenac, Levodopa, Caramazepine Trimethoprim, Aciclovir, Octopamine, Synephrine, Amphetamine, Isoniazid, Norephedrine.	Ascorbic acid for homogenous redox buffering in electrospray ionization-mass spectrometry, S. Plattner, R. Erb, J.P. Chervet, H. Oberacher, Analytical and Bioanalytical Chemistry, 2012, 404(5), 1571-1579	EC1, RC	BDD	OX
2014-06	Amodiaquine, Morphine, Melatonine	Studying the reducing potencies of antioxidants with the electrochemistry inherently present in electrospray ionization-mass spectrometry, S. Plattner, R. Erb, J.P. Chervet, H. Oberacher, Analytical and Bioanalytical Chemistry, 2014, 406(1), 213-224	EC1, RC	GC, BDD, Pt	OX
2017-05	Methanol, Ethanol*	Online Monitoring of Methanol Electro-Oxidation Reactions by Ambient Mass Spectrometry, S. Cheng, Q. Wu, H. D. Dewald, H. Chen, Journal of The American Society for Mass Spectrometry, 2017, 28(6), 1005-1012	RC	Au, Pt, Pt/C (50 w%)	OX
2018-06	Tetrahydroisoquinolines (THIQs)*	Investigations of the Copper-Catalyzed Oxidative Cross-Coupling of Tetrahydroisoquinolines with Diethylzinc by a Combination of Mass Spectrometric and Electrochemical Methods, J. A. Willms, H. Gleich, M. Schrempp, D. Menche, M. Engeser, Chemistry A European Journal, 2018, 24(11), 2663-2668	RC	BDD	OX

EC1= Emitter Cell, this is a special type of cell which is integrated into an AB Sciex ESI spray interface. This device consisted of a cylindrical sandwich assembly containing a planar BDD electrode.

Table 12. Review Articles & Books

#	Compound(s)	Reference	Reactor	WE	Mode
2010-04	Review EC-MS in drug metabolism studies	Online electrochemistry/mass spectrometry in drug metabolism studies: principles and applications, A. Baumann, U. Karst, Expert Opinion on Drug Metabolism & Toxicology, 2010, 6(6) 715-731	RC	Pt, Au, Ag, Cu, GC, BDD	OX, RED
2013-04	Review EC-MS	Recent advances of electrochemical mass spectrometry, P. Liu, M. Lu, Q. Zheng, Y. Zhang, H. D. Dewalda, H. Chen, The Analyst, 2013, 138(19), 5519-5539	RC, SC, u-PC	Pt, GC, BDD, Au, Ag, Cu, Ti	OX, RED
2013-13	Review EC-MS	Life Science Applications of Electrochemistry Coupled to Liquid Chromatography-Mass Spectrometry, H. Oberacher, F. Pittler, LCGC, Special Issues, 2013, 11(4), 26-33	RC, CC, u-PC	Pt, GC, BDD	OX, RED
2014-12	Review EC-MS in metabolism studies	Electrochemistry/Mass Spectrometry as a Tool in Metabolism Studies-a Review, H. Faber, M. Vogel, U. Karst, Analytica Chimica Acta, 2014, 834,9 -21	RC, uPC, SC	GC,BDD, Au, Pt	OX/RED
2015-13	Review Microfluidic electrochemical cells	Miniaturization of electrochemical cells for mass spectrometry, F. T.G. van den Brink, W. Olthuis, A. van den Berg, M. Odijk, TrAC Trends in Analytical Chemistry, 2015, 70, 40-49	RC, CC, u-PC	Pt, GC, BDD, Au, Ag, Cu, Ti	OX, RED
2015-15	Review adduct formation & tagging	Adduct formation of electrochemically generated reactive intermediates with biomolecules, L. Büter, M. Vogel, U. Karst, Trends in Analytical Chemistry, 2015, 70, 74-91	RC	GC,BDD, Au, Cu, Pt	OX
2015-16	Review EC-MS	"Omics" Applications of Electrochemistry Coupled to Mass Spectrometry - A Review, H. Oberacher, F. Pittler, J.P. Chervet, LCGC Europe, 2015, 28(3), 138-150	CC, RC, µ-PC	Pt, GC, BDD, Ti	OX, RED
2017-08	Review EC-MS in xenobiotic metabolism studies	Instrumentation and applications of electrochemistry coupled to mass spectrometry for studying xenobiotic metabolism: A review, L. Portychová, K. A. Schug, Analytica Chimica Acta, 2017, 993, 1-21	RC, SC, u-PC	Pt, GC, BDD, Au, Ag, Cu	OX, RED
2020-04	Book chapter HDX/MS	Chapter 12 - Biophysical mass spectrometry for biopharmaceutical process development: focus on hydrogen/deuterium exchange, G. M. Bou-Assaf, A. G. Marshall, Biophysical Characterization of Proteins in Developing Biopharmaceuticals (2nd ed.), 2020, 333-374	µ-PC1.0-HP	Ti	RED
2020-05	Book chapter HDX/MS	Hydrogen/Deuterium Exchange Mass Spectrometry for the Structural Analysis of Detergent-Solubilized Membrane Proteins, D. P. O'Brien, S. Brier et al., Methods in Molecular Biology, vol 2127, 2020, Humana, New York, NY	µ-PC1.0-HP	Ti	RED

Table 13. Ordering information

Part number	Column description
211.0050	ROXY Exceed with ReactorCell
211.0070	ROXY Exceed EC system with ReactorCell
211.0074	ROXY Exceed EC system with µ-PrepCell 2.0
211.0073	ROXY Exceed EC system for HDX
211.0072	ROXY Exceed EC system for S-S reduction
210.0040	ReactorCell incl BDD, GC, Au, Pt and HyREF
204.4310	µ-PrepCell 2.0 GC/BDD
204.4304	µ-PrepCell SS
206.0037	SynthesisCell with RGC WE-complete
206.0306	SynthesisCell flat smooth BDD working electrode

Fig. 1. Top middle: ROXY Exceed potentiostat. Reactor cells (from left to right): ReactorCell, µ-PrepCell 2.0, µ-PrepCell SS and SynthesisCell.

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