

MUNI
FACULTY
OF MEDICINE

**Mass spectrometry in bioanalytical and
clinical applications**

Habilitation thesis – A commentary

by

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The cumulative habilitation thesis consists of 9 original and 2 review articles published in years 2008–2020 and focuses on the development and applications of mass spectrometry techniques in bioanalytical, medicinal, and clinical chemistry. The entire thesis has been thematically divided into three parts, as follows.

Mass spectrometry hyphenated via an offline interface

Many fields of chemistry, biology, or medicine usually require more than a simple approach in observing critical processes and inferring specific conclusions. Usually, mass spectrometry on its own is not capable of providing answers to complex questions. It is thus beneficial to employ different platform setups to achieve a maximum gain of information entropy.

Mass spectrometry as a tool in identification and characterization

Unambiguous identification of a compound belongs to tasks, which have been haunting chemists for centuries. Any chemical compound may be essentially classified as a known unknown (its structure has already been *de novo* elucidated) or an unknown unknown (no records exist about the structure). Mass spectrometry is a compelling and still readily available technique capable of identifying and characterizing chemical substances, provided they might be ionized. Fragmentation techniques and different types of detection may orthogonal information, leading to minimizing ambiguity in the compound's identity.

Mass spectrometry as a sensitive and specific detector

Recent developments in mass spectrometry allow detection of very low amounts while keeping very high specificity. Theoretical limits of common and abundant mass spectrometric detectors (under optimal conditions) are as low as a few femtograms in a single injection. Additional coupling with a separation technique may enhance the limits even further. Hence, it is reasonable to exploit such a feature in quantitative research, especially when sensitivity and specificity of other methods applied so far may have been reaching their limits.

PES, Ondrej and Jan PREISLER. Off-line coupling of microcolumn separations to desorption mass spectrometry. Journal of Chromatography A 2010, 1217(25), 3966–3977. ISSN 0021-9673. doi:10.1016/j.chroma.2010.02.058 Document Type: Review, IF = 4.194; JCR Category + Category Quartile: BIOCHEMICAL RESEARCH METHODS Q1 + CHEMISTRY, ANALYTICAL Q1; AIS = 0.872

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
60%	40%	80%	40%

PES, Ondrej, Pavla JUNGOVA, Radek VYHNANEK, Tomas VACULOVIC, Viktor KANICKY and Jan PREISLER. Off-Line Coupling of Capillary Electrophoresis to Substrate-Assisted Laser Desorption Inductively Coupled Plasma Mass Spectrometry. Analytical Chemistry. 2008, 80(22), 8725–8732. ISSN 0003-2700. doi:10.1021/ac801036x Document Type: Article, IF = 5.712; JCR Category + Category Quartile: CHEMISTRY, ANALYTICAL Q1; AIS = 1.681

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
70%	20%	60%	20%

JUNGOVA, Pavla, Jarmila NAVRATILOVA, Ondrej PES, Tomas VACULOVIC, Viktor KANICKY, Jan SMARDA a Jan PREISLER. Substrate-assisted laser desorption inductively-coupled plasma mass spectrometry for determination of copper in myeloid leukemia cells. Journal of Analytical Atomic Spectrometry. 2010, 25(5), 662–668. ISSN 0267-9477. doi:10.1039/b919811c Document Type: Article, IF = 4.372; JCR Category + Category Quartile: CHEMISTRY, ANALYTICAL Q1 + SPECTROSCOPY Q1; AIS = 0.816

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
10%	20%	40%	20%

SANDOR, Roman, Adam MIDLIK, Kristyna SEBRLOVA, Gabriela DOVRTELOVA, Kristyna NOSKOVA, Jan JURICA, Iva SLANINOVA, Eva TABORSKA and Ondrej PES (*corresponding author*). Identification of metabolites of selected benzophenanthridine alkaloids and their toxicity evaluation. Journal of Pharmaceutical and Biomedical Analysis 2016, 121, 174–180. ISSN 0731-7085. doi:10.1016/j.jpba.2016.01.024 Document Type: Article, IF = 3.255; JCR Category + Category Quartile: CHEMISTRY, ANALYTICAL Q1 + PHARMACOLOGY & PHARMACY Q2; AIS = 0.618

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
40%	80%	60%	80%

SANDOR, Roman, Jiri SLANINA, Adam MIDLIK, Kristyna SEBRLOVA, Lucie NOVOTNA, Martina CARNECKA, Iva SLANINOVA, Petr TABORSKY, Eva TABORSKA and Ondrej PES (*corresponding author*). Sanguinarine is reduced by NADH through a covalent adduct. *Phytochemistry*. 2018, 145, 77–84. ISSN 0031-9422. doi: 10.1016/j.phytochem.2017.10.010 Document Type: Article, IF = 2.905; JCR Category + Category Quartile: BIOCHEMISTRY & MOLECULAR BIOLOGY Q2 + PLANT SCIENCES Q1; AIS = 0.761

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
40%	70%	90%	50%

SEBRLOVA, Kristyna, Ondrej PES, Iva SLANINOVA, Ondrej VYMAZAL, Jana KANTOROVA and Eva TABORSKA. Seasonal variation in alkaloid composition and antiproliferative activity of *Stylophorum lasiocarpum* (Oliv.) Fedde. *Chemical Papers*. 2015, 69(5), 698–708. ISSN 0366-6352. doi:10.1515/chempap-2015-0083 Document Type: Article, IF = 1.326; JCR Category + Category Quartile: CHEMISTRY, MULTIDISCIPLINARY Q3; AIS = 0.235

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
10%	10%	20%	20%

TABORSKY, Petr, Josef KUCERA, Jan JURICA and Ondrej PES (*corresponding author*). Heavy water enhancement of fluorescence signal in reversed-phase liquid chromatography. *Journal of Chromatography B-Analytical Technologies in the Biomedical and Life Sciences*. 2018, 1092, 7–14. ISSN 1570-0232. doi:10.1016/j.jchromb.2018.05.037 Document Type: Article, IF = 2.813; JCR Category + Category Quartile: BIOCHEMICAL RESEARCH METHODS Q2 + CHEMISTRY, ANALYTICAL Q2; AIS = 0.557

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
60%	60%	80%	50%

PES, O., A. MIDLIK, J. SCHLAGHAMERSKY, M. ZITNAN a P. TABORSKY. A study on bioluminescence and photoluminescence in the earthworm *Eisenia lucens*. *Photochemical and Photobiological Sciences*. 2016, 15(2),

175–180. doi:10.1039/c5pp00412h Document Type: Article, IF = 2.344; JCR Category + Category Quartile: BIOCHEMISTRY & MOLECULAR BIOLOGY Q3 + BIOPHYSICS + CHEMISTRY, PHYSICAL Q3; AIS = 0.623

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
40%	30%	60%	40%

KOSTOLANSKA, Katarina, Ondrej PES, Ondrej ZENDULKA, Jan MACHAL and Jan JURICA. Determination of lansoprazole, 5-hydroxylansoprazole, and lansoprazole sulfone in human plasma for CYP2C19 and CYP3A4 phenotyping. Chemical Papers. 2019, 73(12), 2955–2963. ISSN 2585-7290. doi:10.1007/s11696-019-00682-4 Document Type: Article, IF = 1.680; JCR Category + Category Quartile: CHEMISTRY, MULTIDISCIPLINARY Q3; AIS = 0.222

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
20%	10%	30%	10%

KOSTOLANSKA, Katarina, Lucie NOVOTNA, Eva TABORSKA a Ondrej PES (*corresponding author*). Online solid-phase extraction liquid chromatography-mass spectrometry of hair cortisol using a surrogate analyte. Chemical Papers. 2019, 73(1), 151–158. ISSN 2585-7290. doi:10.1007/s11696-018-0560-1 Document Type: Article, IF = 1.680; JCR Category + Category Quartile: CHEMISTRY, MULTIDISCIPLINARY Q3; AIS = 0.222

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
40%	90%	70%	50%

DEMLOVA, Regina, Miroslav TURJAP, Ondrej PES, Katarina KOSTOLANSKA a Jan JURICA. Therapeutic Drug Monitoring of Sunitinib in Gastrointestinal Stromal Tumors and Metastatic Renal Cell Carcinoma in Adults-A Review. Therapeutic Drug Monitoring. 2020, 42(1), 20–32. ISSN 0163-4356. doi:10.1097/FTD.0000000000000663 Document Type: Review, IF = 3.681; JCR Category + Category Quartile: MEDICAL LABORATORY TECHNOLOGY Q2 + PHARMACOLOGY & PHARMACY Q2 + TOXICOLOGY Q2; AIS = 0.719

Author's contribution:

Experimental work	Supervision	Manuscript	Research direction
10%	10%	10%	10%