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BOOK OF ABSTRACTS

31 March – 2 April 2016
Eger, Hungary
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Dear Colleagues,

European Symposium on Atomic Spectrometry (ESAS) is one of the premium international meetings of scientists to share recent developments, to stimulate contacts and mutual exchange of experiences and ideas as well as to explore new directions and initiate future collaborations in the atomic spectrometry area. Moreover, this conference is intended to stimulate young scientists and PhD students to present their most up-to-date results and to enable passing-on of research experience from generation-to-generation.

In 2016, ESAS is held in Eger at the Eszterházy Károly University of Applied Sciences with the participation of 180 colleagues not only from the main organizing countries - Czech Republic, Germany, Hungary, Poland and Slovakia - but also from Brazil to Iceland and from Canada to Thailand. Similarly to the previous successful conferences, the topics of ESAS cover both fundamental research and practical application aspects of the atomic spectrometric techniques. In total, 46 oral contributions divided into 10 scientific sessions as well as 89 posters will be presented during ESAS 2016. An exhibition of modern atomic spectrometry instrumentation and related sample preparation techniques is also accompanying this scientific event.

I am proud to announce that ESAS 2016 offers the perfect occasion to honor professor Bernhard Welz with the Török Tibor Medal established by the Hungarian Spectrochemical Association in 1999 for his lifetimescientific achievement in atomic absorption spectrometry and for his support to Hungarian spectroscopic research. Professor Welz, who turns 80 this year, is the third German scientist to receive this award. At the same time, the Ioannes Marcus Marci Spectroscopic Society of the Czech Republic would like also to embrace this opportunity to award the 85-year old Tibor Kántor and Gyula Záray, who turns 70 this year, with the prestigious Ioannes Marcus Marci Medal for their outstanding lifetime scientific achievement and for their cohesiverole exercised in the atomic spectroscopic community of Central and Eastern Europe.

On behalf of the Organizing Committee, I wish you a stimulatingand inspiring participation at ESAS2016. Besides the scientific program, I do hope that you will also enjoy the friendly ambience of the picturesque Baroque city of Eger.

VIKTOR G. MIHUCZ
SECRETARY OF ESAS 2016
MARCH 2016
Program of the European Symposium on Atomic Spectrometry, 31 March – 2 April 2016, Eger, Hungary

Conference venue:

Oratorium Artium Pyrkerianum (1st floor), Eszterházy Károly University of Applied Sciences, Eger

Thursday, 31 March 2016

8:00 – 10:15  Registration
10:00 – 10:15  Welcome address and Török Tibor Medal Award Ceremony
11:00 – 11:20  Ioannes Marcus Marci Medal Award Ceremony
11:20 – 11:40  OL-1  Tibor Kántor, András Bartha: Self-absorption effect in inductively coupled plasma atomic emission spectrometry
11:40 – 12:00  OL-2  Gyula Záray, Victor G. Mihucz, Mihály Óvári, Tamás Szigeti, Franco Lucarelli, Frank J. Kelly: Chemical composition and oxidative potential of indoor and outdoor urban aerosol
12:00 – 13:20  Break

Session 1  Trends and new techniques in atomic spectrometry I

Chairperson: Viktor Kanický and Gyula Záray

13:20 – 13:40  OL-3  Zofia Kowalewska, Hanna Laskowska, Maciej Gieroń: Application of HR-CS FAAS to reveal, evaluate and overcome certain spectral events in lead determination in petroleum products
13:40 – 14:00  OL-4  József Posta, István Papp, Dávid Nagy, Csaba Falussy: Atomization of mercury and cadmium compounds under inert high-temperature environment with thermspectrometric method
14:00 – 14:20  OL-5  Aleš Hrdlička, Magda Dvořáková, Pavel Slavíček, Viktor Kanický: Analytical and technical aspects of free discharge end of plasma pencil
14:20 – 14:40  OL-6  Ernest Beinrohr, Lubomir Machynak, Frantisek Cacho: Determination of trace concentrations of chlorides by continuum source high resolution graphite furnace atomic absorption spectrometry

Session 2  Laser spectroscopy I

Chairperson: Margaretha de Loos-Vollebregt and József Posta

14:40 – 15:10  KL-1  Javier Laserna: From the sea bottom to the red planet with laser-induced breakdown spectroscopy
Session 3  
**Laser spectroscopy II**

Chairperson: **Andreas Limbeck** and **Gábor Galbács**

1530 – 1550 OL-7 **Anikó Metzinger**, Éva Kovács-Széles, Gábor Galbács: Development of analytical methods for the determination of Cs, Th and U in nuclear run-off liquid samples by LIBS

1550 – 1610 OL-8 **Winfried Nischkauer**, Frank Vanhaecke, Andreas Limbeck: Self-aliquoting micro-array plates in combination with dried-droplet laser ablation for the quantification of trace elements in whole blood

1610 – 1630 Coffee Break I

Session 4  
**Quality of measurements and metrology and Sample preparation and introduction techniques**

Chairperson: **Alessandro D’Ulivo** and **Gerhard Schlemmer**

1630 – 1700 KL-2 **Viktor Kanicky**, Karel Novotný, Markéta Holá, Michala Vasinová Galiová, Tomáš Vaculovič, Aleš Hrdlička: Recent advances and applications in laser ablation inductively coupled plasma mass spectrometry

1700 – 1720 OL-10 **Stanis³aw Walas**, Natalia Miliszkiewicz, Anna Tobiasz, Emilia Grygo-Szymanko: Calibration approaches in laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS)


1800 – 1830 KL-3 **Ewa Bulska**, Anna Ruszczyńska, Anna Konopka, Eliza Kurek: Investigation of elements bio-transformation in plants via speciation studies

1830 – 1850 OL-13 **David Milde**, Tomáš Pluháček, Martin Kuba: Key challenges in metal impurities determination in pharmaceutical products

1850 – 1910 OL-14 **Aslý Baysal**, Sevilay Tarakei, Ersin Kilic, Ahmet Aköz: Microbial characterization of outdoor samples in smoke and non-smoke areas using VITEK-MS and their effect on human health

1915 – 2130 Poster session (see detailed list at the end of program)

Venue: foyer of Oratorium Artium Pyrkerianum

2030 -2200 **Get-together-Party**– Venue: foyer of Ceremonial Hall (1st floor), Eszterházy Károly University of Applied Sciences

Poster session (see detailed list at the end of program)
Friday, 1 April 2016

Session 5  *Trends and new techniques in atomic spectrometry II*

Chairperson: **Ewa Bulska** and **György Heltai**

8:00 – 8:20 OL-15 **Pierre Masson**: One century of progress for the elemental determination in plants by atomic spectrometry

8:20 – 8:50 OL-16 **Petar Ivanov**, Olaf Schulz, Dirk Wuestkamp: New plasma observation approaches for the analysis of precious metals

8:50 – 9:10 OL-17 **Guilherme L. Scheffler**, Camila A. Martins, Dirce Pozebon: Simple means to enhance robustness in axial view USN-ICP-OES via an additional nitrogen gas stream

9:10 – 9:30 OL-18 **Jan Preisler**, Iva Benešová, Kristýna Dlabková, Tomáš Vaculovič, Viktor Kanický, Antonín Bednařík, František Zelenák: Gold nanoparticle characterization using laser-assisted sample introduction to ICP-MS


9:50 – 10:10 OL-20 **Jürgen Schram**, Uwe Oppermann: The easy way of analyzing oil samples using ICP-OES spectrometry in radial view

10:10 – 10:30 OL-21 **Barbara Wagner**, Zofia Żukowska, Mikołaj Donten, Beata Wrzosek, Anna Lewandowska: LA-ICP-MS imaging data as a support for pigment identification

10:30 – 10:50 OL-22 **Johan Leinders**: Shimadzu’s corporate profile; 140 years of Excellence in Science

10:50 – 11:10 OL-23 **Gregory Lecornet**: Microwave plasma - atomic emission spectroscopy, a revolutionary new technique and plasma source that increases performance while eliminating expensive gas requirements

11:10 – 11:30 Coffee Break II

Session 6  *Trace and ultratrace analysis*

Chairperson: **Maria Goreti R. Vale** and **Tibor Kántor**

11:30 – 12:00 KL-4 **Éva Kovács-Széles**, Tamás Bíró: Application of ICP-MS in origin assessment of nuclear materials

12:00 – 12:20 OL-24 Davide Angelini, Emanuela Pitzalis, **Alessandro D’Ulivo**: Insights into the chemical vapor generation of cadmium at trace levels

12:20 – 12:40 OL-25 **Gábor Galbács**, Ildikó Kálomista, Sára Bálint: On the possibility of the determination of deuterium by ICP-MS

12:40 – 13:00 OL-26 **Michaela Zeiner**, Iva Juranovic Cindric, Boris Majic, Gordana Rusak, Gerhard Stingeder: Effect of ripeness on the accumulation of toxic and essential ultra-trace elements in fruits of *Sorbus Domestica* L.
13:00 – 13:20 OL-27 **Uwe Oppermann, Jan Knoop, Jürgen Schram, Felix Winzheim:** Simultaneous analysis of major-, minor- and trace elements in beer using ICP-OES spectrometry

13:20 – 13:40 OL-28 **Emilia Vassileva, Irena Wysocka:** Determination of trace elements in the open ocean: method validation

13:40 - 14:10 Coffee Break III

**Session 7**  
*Mössbauer spectroscopy and X-ray techniques*

Chairperson: **Michaela Zeiner** and **Ernő Kuzmann**

14:10 – 14:40 KL-5 **Zoltán Homonnay, Ernő Kuzmann, Péter Zsabka, Noémi M. Nagy, József Kónya:** $^{57}$Fe Mössbauer spectroscopic evidence for iron introduction into the interlayer space of montmorillonite

14:40 – 15:00 OL-29 **Ivana Bonková, Marek Bujdoš, Marcel Miglierini:** Characterization of structural positions of iron in biological tissues

15:00 – 15:20 OL-30 **Sebastião da Silva, Luciana Rebelo Guilherme, Aderbal Carlos de Oliveira, Vijayendra Kumar Garg, Attila Lengyel, Roland Szalay, Zoltán Klencsár, Gyula Tolnai, Zoltán Homonnay, Ernő Kuzmann:** Study of carboxylic acid-coated nanomagnetites

15:20 – 15:40 OL-31 **Lukáš Paštěka, Marek Bujdoš, Marcel Miglierini:** Study of steel materials by Mössbauer spectroscopy

15:40 – 16:00 OL-32 **Krisztina Kovács, Ferenc Fodor, Ádám Solti:** Mössbauer spectroscopic study of the oxidation state of iron in plant roots during the iron uptake process

16:00 – 16:20 OL-33 **Felicián Gergely, János Osán, Rainer Dähn, Margit Fábian, Daniel Grolimund, Annamária Kéri, Szabina Török:** Microscale X-ray spectrometry investigation of radionuclide uptake on argillaceous rocks

16:20 – 16:40 OL-34 **Christopher Calam:** Extending the capability of portable XRF into new markets and applications

17:00 - Excursion to Wine Village of Demjén  
*Conference dinner at Crown Wine House - Sponsored by Analytik Jena AG and Shimadzu Europa GmbH*  
*Poster Award ceremony*

**Saturday, 2 April 2016**

**Session 8**  
*Atomic absorption, atomic fluorescence and atomic emission methods*

Chairperson: **Silvia Ružičková** and **Bernhard Welz**

8:00 – 8:30 KL-6 **Gerhard Schlemmer:** Figures of Merit (FOM) and Instrument Performance Verification in Optical Elemental Spectroscopy

8:30 – 8:50 OL-35 **Wiliam Boschetti, Marcelo Orlando, Luíza M.G. Dalagnol, Mariana Dullius, Morgana B. Dessuy, Maria Goreti R. Vale:** Sequential and simultaneous determination of Cd, Cr, Fe and Al in soil samples using HR-CS GF AAS and direct solid sample analysis
Margaretha de Loos-Vollebregt, Guillermo Grindlay, Luis Gras, Juan Mora: A study of carbon-, sulfur- and phosphorus-based charge transfer reactions in inductively coupled plasma atomic emission spectrometry

Katalin Zih-Perényi, Fanni Gyalus, Tamás Szigeti: Determination of trace elements in fuels by microemulsion based GFAAS method

Coffee Break IV

Session 9  Speciation Analysis
Chairperson: Éva Kovács-Széles and Ernest Beinrohr

Witphon Thosaikham, Sujira Maneerat, Piyanete Chantiratikul: Application of ion-paired reversed phase HPLC-ICP-MS for determination of extracellular selenium speciation in selenium enriched L. Rhamnosus culture

Victor G. Mihucz, Éva Sugár, Matheus Lopes, Christina Streli, Gyula Záray: Strategies for identification, quantification and preservation of arsenic species in biological samples

Mehmet Doğan, Mustafa Soylak, Latif Elçi: New trends on the solid phase extraction of inorganic antimony species at trace levels in natural water samples by atomic absorption spectrometry

Camila Corrêa Pereira, Alexander Ossanes de Souza, Emanueli do Nascimento da Silva, Anderson Schwingle Ribeiro, Mariana Antunes Vieira, Solange Cadore: Determination of total and bioaccessible fraction of Ba, Cu, Fe, Mn and Zn in strawberry

Coffee Break V

Session 10  Sample preparation and introduction techniques
Chairperson: Solange Cadore and Mehmet Doğan


Katalin Kovács, Anita Takács, Márk Horváth, Gábor Halász, György Heltai, Zoltán Győri: Acceleration of sequential extraction procedures of potentially toxic element (PTE) content of soils and sediments by sonication

Anna Krejčová: Cleaning procedures and relevance of hair analysis

Saliha Ilican: A comparative study on the optical parameters of sol gel derived different doped ZnO films

Closing ceremony
Poster presentations
Chairperson: Éva Kovács-Széles and Victor G. Mihucz

Atomic absorption, atomic fluorescence and atomic emission methods

P01 **Edina Baranyai**, Edina Simon, Mihály Braun, Béla Tóthmérész, István Fábián: The effect of fireworkon the elemental concentration of dust deposited on tree leaves

P02 **Aslı Baysal**, Suleyman Akman: Peptides coated gold nanoparticles for removal of heavy metals in water samples by graphite furnace atomic absorption spectrometry

P03 Elena Shabunya-Klyachkovskaya, Vasiliy Kiris, **Michail Belkov**, Igor Magalinsky: A comprehensive study of the non-ferrous metals artifacts from the Zapolotski Posad of ancient Polotsk

P04 **Lenka Bendakovská**, Martín Resano, Anna Krejčová, Tomáš Černohorský: Analysis of thallium in spruce needles using solid sampling high-resolution continuum source GF AAS

P05 **Valentina Della Porta**, Emilia Bramanti, Alessandro D’Ulivo, Massimo Onor, Massimo Corsi, Roberto Bianchini: Innovative natural defatting agents: Study of the interaction with leather proteins and monitoring of the environmental impact

P06 **Gabriella Dravecz**, Nikoletta Laczai, Zsuzsanna Szaller, Ivett Hajdara, László Bencs: Solid sampling determination of Mg in LiNbO3 crystals by high resolution continuum source atomic absorption spectrometric method

P07 **Maciej Durkalec**, Jozef Szkoda, Agnieszka Nawrocka, Sebastian Opalinski, Roman Kolacz, Jan Zmudzki: Cadmium in wild boar from areas of industrial activity in Poland

P08 **Jacek Giersz**, Krzysztof Jankowski: An application of the programmable thermostated spray chamber for direct chemical vapor generation in ICP-OES and MIP-OES

P09 **Sándor Harangi**, Zsuzsanna Balogh, István Gyulai, Béla Tóthmérész, Edina Simon: Effects of anthropogenic activities on sediment chemistry in lake Velence (Hungary)

P10 **Attila Kohut**, Gábor Galbács, Zsolt Geretovszky: Characterization of a spark discharge plasma used for copper nanoparticle generation

P11 **Nikoletta Laczai**, Gabriella Dravec, László Kovács, László Bencs: Determination of alkaline elements in yttrium oxyorthosilicate by solid sampling HR-CS-GFAAS

P12 Silvia Ružičková, **Vladislava Mičková**: Evaluation of evaporation process within the frame of optimization of SS-ETV-ICP-OES method

P13 **Petko Mandjukov**, Anna Maria Orani, Eunmi Han, Sabine Azemard, Emilia Vassileva: Calibration and statistical data evaluation in direct solid sampling methods

P15 **Uwe Oppermann**, Jan Knoop, Marion Egelkraut-Holtus, Ludivine Fromentoux, Jürgen Schram: Antimony in breakfast tea – Characterization and quantification of heavy metals in food packaging

P16 Yaroslav Bazel, Rastislav Serbin, **Silvia Ružičková**: Speciation of platinum using various possibilities of analytical signal enhancement. Comparison of AAS and UV-VIS determination of platinum.

P17 **Guilherme L. Scheffler**, Camila A. Martins, Dirce Pozebon: Straightforward determination of U, Th, and Hf at trace levels using ultrasonic nebulization and axial view ICP OES

P18 **Csilla Noémi Tóth**, Edina Baranyai, Sándor Harangi, Zsolt Baranyai, István Fábián: Analysis of gadolinium in protein fractions of human serum spiked with the MRI contrast agent Omniscan

P19 Nil Ozbek, **Gül Sirin Ustabasý**, Suleyman Akman: Direct determination of lead in plastic toys by solid sampling high resolution-continuum source graphite furnace atomic absorption spectrometry

P20 Alexandre de Jesus, Alvaro T. Duarte, Tatiane Pretto, Morgana B. Dessuy, **Maria Goreti R. Vale**: Determination of Na, K, Mg, Ca and Si in biomass samples and their pyrolysis products using HR-CS AAS

P21 Daiane Paula Cunha de Quadros, Mauana Schneider, Eduardo Carasek, **Bernhard Welz**: A novel extraction-based procedure for the determination of cadmium in marine macroalgae by HR-CS GF AAS

P22 Enikő Bitay, Irén Kacsó, Claudiu Tănăselia, Dana Toloman, Ioan Bratu, **Dorottya Nyulas**, Szilamér Pánczél, Erzsébet Veress: Spectroscopic characterization of iron slags from the archaeological sites Brâncovenesci, Călușăreni and Vătava located on the Mureș County sector (Romania) of the Roman Limes.

P23 Mehdi Oubahmane, Abderrahmane Romane, Adil Chahid: Evaluation of heavy metal traces (Pb, Cd and Hg) of some fish by GF-AAS and CV-AAS

P24 Marianna Pozzatti M.S., Alexandre de Jesus, **Maria Goreti R. Vale**: Determination of Cd, Cr and Cu in vegetables of the *Solanaceae* family using high-resolution continuum source graphite furnace atomic absorption spectrometry

P25 Raimundo R. Gamela, Alvaro T. Duarte, Eliana C. G. Barrera, Morgana B. Dessuy, **Maria Goreti R. Vale**: Method development for the determination of Cu and Mn in infant formulas by HR-CS GF AAS using direct solid sample analysis
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*Aurimas Baskevicius*, Simas Butkus, Ona Balachninaite, Domas Paipulas, Valdas Sirutkaitis: Analysis of femtosecond micromachining process in water with laser induced breakdown spectroscopy

**P27**  
*Míchal Brada*, Katarína Skočovská, Pavel Pořízka, David Prochazka, Jan Novotný, Karel Novotný, Jozef Kaiser: Optimization of flat jet nozzle designed for analysis of suspensions containing microparticles

**P28**  
Markěta Tesařová, Marie Šejnohová, Tomáš Žíkmund, Pavel Pořízka, David Prochazka, Karel Novotný, **Jozef Kaiser**: Combination of laser-induced breakdown spectroscopy and X-ray micro computed tomography for high-resolution elemental mapping

**P29**  
Katarína Skočovská, Jan Novotný, David Prochazka, Pavel Pořízka, Karel Novotný, **Jozef Kaiser**: Optimization of liquid jet system for laser-induced breakdown spectroscopy analysis

**P30**  
*Jakub Klus*, Pavel Pořízka, David Prochazka, Jan Novotný, Karel Novotný, Jozef Kaiser: Multivariate approach to study of element association in sandstone-hosted uranium ores

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Emanuela Grifoni, *Stefano Legnaioli*, Giulia Lorenzetti, Stefano Pagnotta, Vincenzo Palleschi: The SHREDDERSORT Project: LIBS and ANN for selective recovery of non-ferrous metal automotive shredder

**P32**  
Maximilian Bonta, Hans Lohninger, Balazs Hegedus, *Andreas Limbeck*: Laser-based methods for the laterally resolved elemental analysis of biological samples

**P33**  
Pavel Pořízka, *Jakub Klus*, David Prochazka, Gabriela Vítková, Jan Novotný, Karel Novotný, Jozef Kaiser: Assessment of the most effective part of Echelle LIP spectra for classification purposes; for further use of Czerny-Turner spectrometer

**P34**  
Pavlína Škarková, Karel Novotný, Přemysl Lubal, Alžběta Jebavá, Pavel Pořízka, David Prochazka, Aleš Hrdlička, Jozef Kaiser: Laser-induced breakdown spectroscopy 2D distribution mapping of quantum dots

**P35**  
Lucia Sládková, Pavlína Škarková, Michaela Remešová, Pavel Pořízka, David Prochazka, Karel Novotný, Ladislav Čelko, Jozef Kaiser: Improvement of the laser-induced breakdown spectroscopy method sensitivity by combination of Ag-nanoparticles and vacuum conditions

**P36**  
*Michaela Tvrdoňová*, Tomáš Vaculovič, Viktor Kanický, Zuzana Čadková, Jiřina Száková, Pavel Tlustoš, Vítězslav Otruba: Accumulation of Pb, Cd, Zn and Cu in tapeworm tissue imaged by LA-ICP-MS method

**P37**  
Gabriela Vítková, Pavel Pořízka, David Prochazka, Jakub Klus, Karel Novotný, Jozef Kaiser: Optimization of LIBS measurement parameters via multivariate chemometrics for the classification purpose

**P38**  
*Magdalena Zvolska*, Tomas Cemohorsky, Miloslav Pouzar: Determination of cadmium and lead in biological fluids using laser-induced breakdown spectrometry
**Mass spectrometry, X-ray spectrometry and Mössbauer spectroscopy**

P39 **Jitka Hegrová**, Roman Ličbinský, Oliver Steiner, Walter Goessler, Jiří Faimon: Element determination in different size of airborne nanoparticles by ICP-QQQ

P40 **Anna Konopka**, Dominic Winter, Witold Konopka, M. Estela del Castillo Busto, Susana Nunez, Heidi Goenaga-Infante, Paola Fisicaro, Ewa Bulska, Wolf D. Lehmann: Novel full-length selenoprotein standards for quantitative proteomics

P41 **Agnieszka Nawrocka**, Maciej Durkalec, Jozef Szkoda and Andrzej Posyniak: Determination of toxic and essential elements in seafood by inductively coupled plasma mass spectrometry

P42 **Jan Patočka**, Anna Krejčová, Lenka Bendakovská, Tomáš Černohorský: Development of the ETV-o-TOF-ICP-MS technique and its comparison with the o-TOF-ICP-MS technique in analysis of thallium in spruce needles

P43 **Tomáš Pluháček**, Jaroslav Hanzal, Jiří Hendrych, David Milde: Heavy metals and sulfated ash testing: an alternative approach

P44 **Éva Cseperke Vizsolyi**, Péter Dobosy, Imre Varga, József Varga, Gyula Zárây: Degradation of chlorobenzene compounds in groundwater by ferrate treatment

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CURRICULUM VITAE AND PLENARY LECTURE ABSTRACT OF LAUREATE OF TÖRÖK TIBOR MEDAL OF HUNGARIAN SPECTROCHEMICAL ASSOCIATION
Curriculum Vitae of Bernhard Welz

Bernhard Welz received his PhD in Chemistry from the University of Stuttgart in Germany in 1966 and started his career as an application specialist for atomic absorption spectrometry at Bodenseewerk Perkin Elmer, Germany, in 1967; later he became the head of the Applied Research Department, a position that he held until his forced early retirement in 1998. In 1999, he moved to Brazil first as a Visiting Professor at the Federal Universities of Santa Catarina and of Bahia and then as a voluntary professor at the Federal University of Santa Catarina in Florianópolis, where he is still active.

In 1967, Bernhard Welz participated in the 1st Atomic Absorption Symposium in Prague, Czechoslovakia, met with Boris L’vov and Hans Massmann and decided to devote his research to graphite furnace AAS (GF AAS). He pioneered the introduction of the first commercial graphite furnace in 1970 and continued promoting all the improvements of this technique, such as the STPF concept in close cooperation with Boris L’vov, Hans Massmann and Walter Slavin. In 1986, he proposed together with his coworker Gerhard Schlemmer the palladium and magnesium nitrates modifier as a “universal modifier” for GF AAS, which became the third most cited manuscript of Spectrochimica Acta Part B. In the late 1980s and early 1990s, he devoted himself to the coupling of flow injection techniques to flame, graphite furnace and vapor generation AAS in close cooperation with Zhao-lun Fang. In the late 1990s, he started to work with High-resolution Continuum Source Atomic Absorption Spectrometry in close cooperation with the group of Helmut Becker-Ross, research that was continued and intensified after his move to Brazil. Using this new technique, he also intensified his research about direct solid sample analysis with GF AAS and found that a wide variety of samples could be analyzed without interference using calibration against aqueous standards. During the last years, he dedicated most of his research to the determination of non-metals, particularly the halogens, using the same equipment for High-resolution Molecular Absorption Spectrometry.

Bernhard Welz was also organizer and co-organizer of 25 international conferences about Atomic Spectrometry. In 1981, he created the Colloquium Atomspektrometrische Spurenanalytik (CAS), which was later united with a similar conference organized by Klaus Dittrich in the former GDR and re-named Colloquium Analytical Atomic Spectrometry (CANAS). In 1988, he organized in cooperation with Adilson J. Curtius the first Rio Symposium on Atomic Spectrometry, a conference, which is nowadays considered the leading conference on atomic spectrometry in Latin America. He also succeeded to get the Colloquium Spectroscopicum Internacionale, CSI XXXVII to Brazil, which he organized jointly with Reinaldo C. Campos in Buzios, RJ.


In 1988, he received the Ioannes Marcus Marci medal from the Bohemian and Slovakian Spectroscopic Societies and in 2006 the Clemens-Winkler medal of the German Chemical Society. Bernhard Welz has about 280 publications in international scientific journals, almost 10,000 citations and a Hirsch index of 54.
FROM EVIL TO BLESSING: MOLECULAR ABSORPTION SPECTRA IN GRAPHITE TUBE ATOMIZERS

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Since the introduction of the first commercial graphite tube furnace (GF) for atomic absorption spectrometry (AAS) in 1970, the appearance of molecular absorption spectra caused by matrix constituents was considered the most notorious spectral interference in GF AAS. The spectra of gaseous diatomic molecules, such as PO, NO or CS, exhibit a pronounced fine structure, which could not be handled by the background correction (BC) systems available at that time, including Zeeman-effect BC. The result was a significant distortion of the analyte signal, which caused erroneous results when compared with matrix-free calibration standards. Only high-resolution continuum source AAS (HR-CS AAS), which was introduced commercially at the beginning of this century, could finally solve this problem.

Independent of that, the spectra of diatomic molecules were investigated since the 1970s for their applicability to determine non-metals, such as phosphorus, sulfur and the halogens via molecular absorption spectrometry (MAS) in flames and furnaces. Some 30 papers appeared about the subject in the following years [1]; however, the equipment available at that period (conventional line-source atomic absorption spectrometers) did not support this idea, and the area was abandoned in the 1990s. The introduction of commercial equipment for HR-CS AAS early in this century gave a new impetus to the idea, and the group of Becker-Ross in Germany published a whole series of papers, which are summarized in a recent Review article [2], pioneering the revival of the technique. Due to the high-resolution monochromator, the rotational fine structure of the molecular absorption spectra is well resolved, and due to the use of a continuum radiation source and a CCD array detector, each of the lines can be used for analytical purposes, and the valleys between the lines are available for background correction.

There are molecules that form spontaneously in the graphite furnace under favorable conditions, such as PO, NO or CS, whereas others, particularly those for the determination of the halogens, have to be “synthesized” by the addition of an appropriate “molecule-forming reagent” in excess. We started our research in this area a decade ago with phosphorus, comparing molecular with atomic absorption and came to the conclusion that in many cases AAS is the method of choice. We continued with sulfur using the CS molecule with some success; however, the molecule formation depended on the availability of reactive carbon in the atomizer. We finally decided to go to the SnS molecule, which formed upon the addition of an excess of tin, and which worked out very well. Most of our recent research was focused on the determination of the halogens, mostly F, Cl and Br. We have chosen the calcium mono-fluoride molecule CaF and the strontium mono-chloride SrCl, which are forming upon the addition of a large excess of a calcium or strontium solution, respectively, at high temperature (≥ 2000 °C) upon volatilization in the GF. The graphite furnace also makes possible the direct introduction and analysis of solid samples, avoiding any unnecessary sample preparation, such as acid digestion or alkaline fusion. Among the matrices investigated with this technique are toothpaste, plant material, mineral coal, copper concentrate, air particulate matter and eye shadows. All of these materials were analyzed using aqueous standards for calibration, demonstrating the robustness of the method.

Acknowledgments: CNPq, CAPES, INCT E&A, Analytik Jena
References
CURRICULUM VITAE AND LECTURE ABSTRACTS OF LAUREATES OF IOANNES MARCUS MARCI SPECTROSCOPIC SOCIETY
Curriculum Vitae of Tibor Kántor

Tibor Kántor graduated from the Technical University of Budapest as chemical engineer in 1953. His first employment was at the Central Institute of Physics, Department of Spectroscopy from 1953 to 1959, and then he received a status as research coworker in the Academic Research Group of the Technical University of Budapest, Department of General and Analytical Chemistry. From 1970, he got the rank of senior research worker and was nominated as the leader of the Spectrochemical Research Group until 1990, when he was sent to retirement officially.

However, from the next year, 1991, he continued the research work at the Eötvös Loránd University, Department of Inorganic and Analytical Chemistry and further on at the Department of General and Inorganic Chemistry (1998-2006) being financed by the Hungarian Research Foundation. Presently, he is honorary coworker at the Spectroscopic Laboratory of Geological and Geophysical Institute of Hungary.

Regarding his scientific degrees, he received doctor technicus (MSc) title in 1965, candidate degree (PhD) in 1976 and doctor of science degree (DSc) in 1987. He received the Professor title from the Technical University of Budapest in 1990.

Longer stipendiums in abroad were 12 months stay at the University of Houston (Texas), 1973-74 and 6 months stay at the University of Florida (USA), 1981-82.

Major research field has been the Analytical Atomic Spectroscopy and the main interest was focused on high temperature chemical processes in spectroscopic sources. The following scientific results might be considered significant during his career:

1. Role of the vaporization process in the analytical function of emission spectroscopy (1969-1974);
2. Introduction of the graphite-arc vaporization (dispersion) technique for sample introduction into flames (1973);
3. Introduction of the laser ablation technique for sample introduction into flames (1976);
4. New interpretation of the releasing effect in flame spectrometry (elimination of aluminium interference on calcium determination) (1987);
5. Introduction and studies of halogenation reactions with halocarbon vapors in d.c. arc (1980), flame (1983), graphite furnace (1983), ICP (1994) and combinations of these sources.

He published 124 scientific papers and 9 book chapters (one in English), the number of citations to his articles is about 980. He is a member of the Editorial Advisory Board of the periodical Spectrochimica Acta Part B from 1987.

He was elected chairman of the Spectrochemical Association of the Hungarian Chemical Society for two years (1995 and 1996). He was granted with the Tibor Török Award by the Hungarian Spectrochemical Association (2002), with the Jerzy Fijalkowski Award by Committee of Analytical Chemistry of Polish Academy of Sciences (2009) and with the Nicolaus Konkoly Thege Award by the Slovak Spectroscopic Society (2010).
SELF-ABSORPTION EFFECT IN INDUCTIVELY COUPLED PLASMA
ATOMIC EMISSION SPECTROMETRY

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The emission of spectral lines in the function of atomic and ionic concentration was studied from the beginning of last century and principally two ways were followed in the theoretical treatment. One of them was the physical theory based on the “curve of growth” concept and the other was the phenomenological theory in the sense that it expresses mathematically the results of observations without paying detailed attention to their fundamental significance. The latter theories have provided practically applicable analytical functions to different excitation sources, and extension toward inductively coupled plasma atomic emission spectrometry (ICP-AES) was aimed at presently.

Conceptually, an up to date ICP-AES instrumentation was applied which made possible the radial and axial viewing of the plasma, as well, the measurement of line peak height and line peak area intensities. These requirements were satisfied by the Perkin-Elmer Optima 8300 DV ICP-AES spectrometer equipped with echelle grating and segmented-array charge-coupled device (SCD) detector. The intensities were measured in “auto-read” mode (5 points/peak), the software selected the integration time and number of integrations automatically applying a short time pre-detection. The integration time multiplied with the number of integrations is equal with the “read time”. The counts accumulated are divided by the read time to provide the intensity in cps unit. Similar instrumentation was used earlier in the studies of self-absorption effect by Chausseau et al., who applied polynomial regression for fitting the calibration curves [1].

Two resonance atomic and ionic lines of Cd and Mg were studied, the concentration range was extended up to 2000 mg/L. At the varying analyte concentration, constant matrix concentration of 10000 mg/L Ca was ensured in the pneumatically nebulized solutions. As the continuity of the earlier results the following equation could be experimentally verified [2]:

\[ \text{I} = ac \exp(-\beta c + kc^2) \]

where \( I \) is net line intensity, \( c \) is concentration and \( a, \beta \) and \( k \) are constants. The term, \( kc^2 \), has significance only above 100 mg/L concentration and it results in a decrease of the effect of self-absorption on the shape of the analytical curve at very high concentrations. Its physical meaning is related to the emission and absorption line profiles and to the features of the spectral line detection. The width of the pixel aligned to the center of emission line is considerably larger than the width of the absorption line. With increasing concentration more and more parts of the internal areas of the line wings are measured which are less intensively absorbed than the line center.

References

The presentation is supported by the Per-Form Hungaria Kft.
Curriculum Vitae of Gyula Záray

Gyula Záray obtained his PhD degree in Chemistry in 1980 at Eötvös Loránd University (ELTE). In 1995 he obtained the Doctor of Science degree of the Hungarian Academy of Sciences (HAS). He has been professor with habilitation at ELTE since 1996. He was head of the Laboratory for Instrumental Analysis at the Research Institute of Non-ferrous Metals in Budapest between 1982 and 1990, then, he became staff member of the Department of Inorganic and Analytical Chemistry of ELTE. He was vice-dean of the Faculty of Sciences of ELTE between 1994 and 2001.

In 1996, he was elected head of the Department of Chemical Technology and Environmental Chemistry of ELTE. He was head of the Joint Research Group of Environmental Chemistry of HAS and ELTE between 1999 and 2006. He has been director of the Hungarian Satellite Centre of Trace Element Institute for UNESCO since 2000. In 2004, he became head of Department of Inorganic and Analytical Chemistry of ELTE. In 2005, he founded - and still presides - the Cooperative Research Centre of Environmental Sciences for ELTE, financially supported by the Hungarian Government and European Union. Currently, he is also head of the Environmental Chemistry and Bioanalytics Research Group at ELTE. In 1985, he was granted with Humboldt fellowship, and he spent 2 years at the Institute of Spectrochemistry and Applied Spectroscopy in Dortmund, Germany. In 1997, he was granted in Hungary for 4 years with Széchenyi fellowship. In 2001, he was awarded with the Pro Universitate award by ELTE. In 2002, he was honored with the commemorative medal of the Technical University of Košice. He was visiting professor in Sapporo (Japan) during 5 months in 2004. In 2004, he was honored with the Golden Cross of Merit of the Republic of Hungary. Hungarian Chemical Society awarded him with the Than Károly award in 2007. Hungarian Spectrochemical Association honored him with the medal of his mentor, Tibor Török in 2015.

Since 1991, he has been the supervisor from the Hungarian side of the Hungarian–Italian Symposium on Spectrochemistry, now in its 15th edition. He organized 4 successful scientific conferences in Hungary, namely 8th Solid Sampling Spectrometry Colloquium in 1998, 6th European Furnace Symposium and 11th Solid Sampling Symposium with Atomic Spectrometry in 2004, 11th International Conference on Total Reflection X-ray Fluorescence Spectrometry and Related Methods in 2005 and Colloquium Spectroscopicum Internationale XXXIV in 2009. He was the European editor of Applied Spectroscopy Reviews between 2004 and 2015. He has been member of the Editorial Board of Microchemical Journal. His research interests focus on the development of solid sampling spectrometric methods for investigation of ceramics; investigation of heavy metal uptake, accumulation and translocation processes in plants; biomonitoring of surface waters; chemical characterization of biofilms; determination of pharmaceutical residues in waste, surface and drinking water, speciation of toxic elements in airborne particulate matter, soil, sediment and food; assessment of oxidative potential of fine particulate matter. His international scientific activities included cooperation with Istituto Superiore di Sanità (Rome, Italy), Friedrich Schiller University (Jena, Germany), University of Vienna (Austria), Hacettepe University (Ankara, Turkey), Lisandro Alvarado Central-occidental University (Barquisimeto Venezuela), Bergen University College (Norway), University of Antwerp (Belgium) and China University of Geosciences (Wuhan, China). He authored 210 SCI articles, seven book chapters and published one book in Hungarian on Instrumental Analysis as well as one in English on analytical techniques for Clinical Chemistry. His total number of independent citations is 2010 and his Hirsch-index is 25 as of February 2016.
CHEMICAL COMPOSITION AND OXIDATIVE POTENTIAL OF INDOOR AND OUTDOOR URBAN AEROSOL

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The urban atmosphere is continuously affected by emission of gaseous and particulate phase contaminants of anthropogenic arising from both stationary (power plants, industries, incinerators, and residential heating) and mobile sources (road traffic). Moreover, people spend the majority of their time in enclosed spaces. Reactive oxygen species (ROS) play an important role in physiological processes as well as in atmospheric chemistry. In biology, ROS comprise a wide range of oxygen-centered and related free radicals, ions and molecules. Upon deposition or formation in the lung, ROS can cause oxidative stress, cell death and biological aging. When particles containing transition metals are inhaled, they can undergo Fenton-like reaction, resulting in the production of ROS in vivo. Biosurfaces such as fluid films containing antioxidants for example ascorbic acid, reduced glutathione, uric acid and α-tocopherol scavenge ozone and ROS.

A comprehensive 3-year long chemical characterization and oxidative potential (OP) assessment of PM2.5 was carried out in modern working environments equipped with heating, ventilation and cooling systems as well as at an urban site characterized by heavy vehicular traffic in Budapest, Hungary. Indoor and concomitantly sampled outdoor samples were taken in the frame of the EU collaborative project, called OFFICAIR. Chemical analyses included the determination of the concentration of trace elements, major water-soluble inorganic ions and carbonaceous fractions (total carbon, water-soluble organic carbon, organic carbon, elemental carbon). The OP of PM2.5 was assessed by antioxidant depletion using a synthetic respiratory tract lining fluid containing ascorbate, reduced glutathione and urate.

The aims of this study were to (i) characterize indoor and outdoor urban PM2.5 through its mass concentration and chemical composition (trace elements, water-soluble inorganic ions, carbonaceous fractions); (ii) measure the OP of the collected particles; and (iii) study the seasonal variations and changes in the chemical composition and oxidative potential of PM2.5 collected for 36 months. Furthermore, the link between particulate OP and the concentration of the PM constituents was investigated. The main outcomes of this comprehensive study will be reviewed during the presentation.
ABSTRACTS OF KEYNOTE LECTURES
Laser-induced breakdown spectroscopy (LIBS) constitutes one of the most active research fields in analytical science. Among several important features, ability for adaptation to radically different scenarios constitutes its most valuable asset. For instance, technology based on LIBS has been developed for sub-sea operations and for planetary exploration, two extreme environments that require analytical solutions not available for most measurement techniques. In this talk, a discussion will be presented on the challenges represented by these analyses and the solutions envisaged using advanced LIBS approaches.
Laboratory of Atomic Spectrochemistry, LAS, (Faculty of Science, Masaryk University) was established in 1997. Since its beginning, LAS has been focused *inter alia* on research of interaction of laser radiation with matter in terms of spectrochemical analysis, and for the need of elemental analysis of solids. As regards nature of analysed objects, research and development is involved in spatially resolved analysis of soft and hard biological tissues, such as thin sections of tumours, tapeworms and plants, teeth, urinary calculi and bones. Analysis of tissues and/or cultivated cells by LA-ICP-MS is attempted for purpose of monitoring the penetration of candidate anti-cancer drugs into cancer cells and to study mechanism of action. Local microanalysis of selected spots as well as elemental mapping of areas of interest in geological samples is performed by means of LA-ICP-MS and LIBS. Archaeological samples, such as glass artefacts, are investigated and provenance analysis of obsidian tool and raw materials is performed. Molten LiF/NaF-induced corrosion of candidate structural alloys for nuclear power stations is studied by LA-ICP-MS. Besides LA-ICP-MS, laboratory-made LIBS facility in single- and double-pulse implementation is used in the analysis of some of above materials, for which contents of elements of interest are above detection limits of LIBS. The LIBS facility offers promising and fast alternative to other detection techniques in detection of nanoparticles and quantum dots.

**Acknowledgment**

This work was supported by European Regional Development Fund project CEITEC (CZ.1.05/1.1.00/0.20068).
Atomic and mass spectrometry are considered to be very useful for the investigation of the elemental as well as isotopic composition of e.g. plants and animal tissues, as well as the food products of various origin. Several analytical procedures, including biological and chemical examination were evaluated towards investigation of the elements bio-transformation via examination of the presence of specific compounds in plants tissues. Selected plant species, namely *Allium cepa* L. was used as a potential source of the functional food. This was due to the fact, that several plants exhibits the ability to accumulate various compounds, those considered as essential for living organism or those known as toxic. Therefore a lot of attention is focused on the investigation of the process ongoing in plants tissues and cells when they are exposed to the enhanced amounts of chemical species in environment.

The aim of the study was to identify various chemical species in onions (*Allium cepa* L.) grown hydroponically or in soil support and in particular to understand the processes of its biotransformation in plants exposed to controlled conditions of cultivation. The determination of the elemental composition of tissues was used for the evaluation of the transport efficiency of selected species in plants, all towards understanding its respond to the environmental conditions. Chromatographic techniques coupled to ICP-MS were used to identify chemical forms of the elements of interest. In order to evaluate the validity of the developed analytical procedures as well as to assure the accuracy of the results, the matrix matched certified reference materials were selected and their usefulness were proved via the quality assurance procedures.

**Acknowledgements**

Financial support from National Centre of Science (NCN, Poland), for the project „Investigation of chemical and biological processes of selenium biotransformation in selenophilic plants and probiotic bacteria towards their application as functional food”, 2012/05/B/ST4/01219 is gratefully acknowledged.

The study was carried out at the Biological and Chemical Research Centre, University of Warsaw, established within the project co-financed by European Union from the European Regional Development Fund under the Operational Programme Innovative Economy, 2007 - 2013.
Illicit trafficking of nuclear and other radioactive materials has emerged as a truly international problem and an indeed dangerous threat to international security. The problem of theft or loss of nuclear materials has affected countries on all five continents proving once again the international scale of this issue. Concerns about nuclear smuggling resulted in the development of a relatively new field known as nuclear forensics.

Nuclear forensics is the analysis of nuclear materials recovered from e.g. the capture of unused nuclear materials or radioactive material to provide evidence for determining the history of the sample material. It contributes significantly to the identification of the sources of the materials and the industrial processes used to obtain them.

The importance of nuclear forensics has increased in the last decades after the decomposition of Soviet Union due to the strengthening of smuggling of nuclear materials (uranium oxide pellets, metallic uranium, uranium ore concentrates, etc.). Therefore, nuclear forensics is an essential technology for control on the transfer of nuclear material and prevention or prosecution of the illicit trafficking of nuclear materials.

Measurement of some characteristic parameters of nuclear materials with unknown origin can be utilized for their identification and characterization. Such analytical parameters sufficient for identification of nuclear material including isotopic composition of uranium, morphology features (e.g. surface roughness), age or production date and impurity levels (rare earth elements and other elements in specific pattern as a fingerprint), or stable isotope ratios.

For precise analysis of these parameters and to the origin assessment of these materials mass spectrometric techniques are basic methodologies. Commonly used mass spec techniques in the field are the thermal ionization mass spectrometry and the secondary ionization mass spectrometry, however inductively coupled plasma mass spectrometry is also often used because it is a good compromise and effective technique to find the answers to the questions of nuclear forensics. To the precise isotope ratio measurements mainly sector field instruments (both single and multi collector ones) are applied. To obtain the highly requested and expected accuracy and precision of the measurements (less than 1% combined uncertainty in isotope ratios) is a challenge.

In this presentation a review of the techniques, methods developed for forensic analysis and results obtained in inter-laboratory comparisons will be shown.
57Fe MÖSSBAUER SPECTROSCOPIC EVIDENCE FOR IRON INTRODUCTION INTO THE INTERLAYER SPACE OF MONTMORILLONITE

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In our previous work [1] we have reported preparation of Fe-montmorillonite by reacting montmorillonite with FeCl3 in acetone. These samples proved to be efficient Lewis catalysts in acylation of aldehydes. In the sample treated with FeCl3, an increase of the basal spacing of montmorillonite was found by XRD, while a new magnetically split component assigned to Fe3+ incorporated within the interlayer regions of montmorillonite showed up in the low temperature Mössbauer spectra. The Mössbauer parameters observed were close to those of iron-oxyhydroxides, so the possible presence of some kind of nanoparticles was also suggested.

The aim of the present work was to elucidate whether all the FeCl3 used for the treatment gets intercalated in the interlayer space of montmorillonite or there may be isotope exchange at regular octahedral sites. Octahedral Fe3+ and Fe2+ always occur in natural montmorillonite. In order to observe separately the natural iron content of montmorillonite and the iron introduced from FeCl3, we applied FeCl3 prepared from isotopically enriched (95%) 57Fe for the treatment of montmorillonite. Since the abundance of 57Fe in natural iron is only 2.17%, in this experiment, Mössbauer spectroscopy can preferentially monitor the fate of 57Fe originated from 57FeCl3, and the signal of the naturally contained iron becomes negligible in the spectra. The 20K Mössbauer spectra of montmorillonite treated with 57FeCl3 in acetone revealed only magnetically split subspectra with parameters corresponding to those assigned to Fe3+ species intercalated between the layers in iron exchanged montmorillonite, showing an evidence for the introduction of iron into the interlayer space of montmorillonite.

References

Acknowledgements
The financial supports from the OTKA (No T043687 and No K115913) grants are acknowledged.
FIGURES OF MERIT (FOM) AND INSTRUMENT PERFORMANCE VERIFICATION IN OPTICAL ELEMENTAL SPECTROSCOPY

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Analytical Figures of Merit (FOM) [1-3] is the performance characteristic of an analytical determination. They can be used to select between potentially useful methods and to evaluate or optimize a method that is already in use. FOM are the base for instrument specifications for manufacturer and user and are aspects of central importance for method validation and data reporting for an analytical measurement. The importance of Analytical Figures of Merit is generally accepted.

FOM are based on instruments’ response to a mass or concentration of analyte-elements in unknown samples, reference solutions or blanks. They are expressed in intensity units, absorbance, characteristic mass etc., and they provide information on the dynamic working range of the application. The repeatability at the edges of the working range as well as in the optimal working range will define limits of detection and quantitation as well as the repeatability of the measurement as a function of the analyte concentration. Freedom from interferences and long term stability provide information on the accuracy and ruggedness of the method and, combined with the repeatability, on the trueness of the result. FOM is used in almost all analytical reference and standard methods published by ISO, EN, EPA etc. and a part of these data is controlled and documented in long-term performance quality control (Shewhart) charts.

FOM are clearly defined and partly based on mathematical and statistical models. The figures, however contain as well important information on the total analytical process as they express a chemical (analytical) or technical (instrumental) “situation”. This link between statistical data and possibly required action for improvement of the situation is very seldom described in the literature.

In this lecture a general overview over FOM and their significance for instrumental parameters and other analytical parameters will be given. Examples from the fields of AAS, AFS and ICP-OES will describe how data, obtained from statistical models, help to evaluate instrumental methods and contribute to identify non-optimized situations.

References
ABSTRACTS OF ORAL CONTRIBUTIONS
APPLICATION OF HR-CS FAAS TO REVEAL, EVALUATE AND OVERCOME CERTAIN SPECTRAL EVENTS IN LEAD DETERMINATION IN PETROLEUM PRODUCTS

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Since the commercial introduction in 1923, tetraalkylleads (TEL) have been widely applied as antiknock agents and have caused significant contamination of environment all over the world, including Greenland snow and high alpine sites. At present the addition of TEL to automotive gasoline is forbidden in many countries, however, it is still applied in production of aviation gasoline. Petrol of type 110LL (blue) and petrol of type 91/115 (green) can contain up to 560 and 850 mg L⁻¹ of Pb, respectively. On the other hand, in some catalytic processes the admissible lead content in raw material is at the level of µg L⁻¹.

The main aim of this work was investigation of spectral effects in lead determination using high-resolution continuum source flame atomic absorption spectrometry (HR-CS FAAS). Among others, the absorption by OH molecule has been considered. The molecule, present in the air-acetylene flame, generates fine-structured bands corresponding to the electronic transition between the X²Π and the A²Σ⁺ states [1]. Until now, the effect of OH absorption on the Pb determination has been reported only once and for aqueous solutions analysis [1].

Two lines of Pb have been studied (217.000 nm and 283.306 nm), as well as various options of baseline fitting and background correction (iterative background correction, reference pixels application, least squares background correction). The samples of different hydrocarbon composition were analyzed. For higher Pb concentration level the obtained results can be related to the results of alternative methods (wavelength dispersive X-ray fluorescence and/or titration with iodine mono-chloride).

The results of the investigation will be applied to establish conditions for accurate Pb determination using both HR-CS FAAS and conventional line source FAAS.

The feasibility and usefulness of internal standard application in Pb determination using HR-CS FAAS will be evaluated.

References
ATOMIZATION OF MERCURY AND CADMIUM COMPOUNDS UNDER INERT HIGH-TEMPERATURE ENVIRONMENT WITH THERMOSPECTROMETRIC METHOD

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Thermospectrometry, a new and unique material testing and analytical method has been developed by combining thermal analysis with atom and molecule spectrometry. The central unit of the method is a stationary furnace that can be heated up to 1700 °C. Nanoparticles of solid, liquid or gaseous samples travel upwards between the two heated walls of the furnace placed 10 mm from each other, where conversion and decomposition processes occur separately in time and space according to the thermal properties of substances. These processes were followed by vertical scanning with narrow light beam of hollow cathode lamp of atomic absorption spectrometer.

Atomization of pseudohalide mercury salts (potassium diiododibromo mercurate(II), mercury(II) cyanide and thiocyanate) and mercury(II) homologues (mercury(II) formiate, acetate and propionate) were studied at various (150 – 900 °C) temperature of the stationary furnace. On the basis of the shape and appearance of thermospectrograms the atomization of mercury compounds at low temperature (150 – 300 °C) take place by significantly different way and rate.

We found that in the thermospectrometer the atomization of cadmium compounds follows at least two different reaction courses. At lower temperatures (650–700 °C) a slower mechanism is dominant at higher regions of the furnace, while at 800 °C a faster mechanism demanding less residence time in the furnace becomes dominant. Under inert atmosphere the degree of atomization strongly depends on the thermal properties of substances.

References
Plasma pencil has been employed as an alternative excitation source for atomic emission spectroscopy determination of elemental contents in solutions [1, 2]. The new arrangement of the discharge tube enables to measure spectra from the free discharge end without shielding by the quartz wall. Most intensive atomic spectra can be recorded as close as possible to the ground electrode but it is also possible to record the plasma tip radiation in the range of about 0-10 mm from the ground electrode or as long as the discharge tip is formed behind the ground electrode.

The pencil sustainability and stability were tested under various operating conditions. Carrier gas and plasma gas flow rates as well as forwarded power were changed and spectra of selected elements were recorded in order to yield best signal to backgroud ratio and discharge stability. It has been found that intensities of some atomic lines increase with decreasing plasma gas flow rate, increasing carrier gas flow rate and slightly with increasing forwarded power up to 180 W in continuous mode. The pulsed mode has not been tested [2].

As in our previous studies elements of first two groups of the periodic table, zinc and copper were tested. In some cases the sensitivity increased by one order of magnitude. Calibration dependences in the range of 0.1 – 10 mg × L⁻¹ were then measured. Also matrix effects similar to those in the previous arrangement were observed. On the other hand, electronic excitation temperature from argon atomic lines, rotational temperature from OH lines and electron number density do not significantly change as a result of mixing argon with ambient air.

Matrix effects by alkali salts were also observed but not eliminated under any operating conditions. Preliminary experiments rather show that the relative decrease of the analyte lines intensities in presence of an alkali salt is preserved.

Acknowledgements
The work was supported by the European Regional Development Fund project “CEITEC” (CZ.1.05/1.1.00/02.0068) and by the project CZ.1.05/2.1.00/03.0086 funded by European Regional Development Fund and project LO1411 (NPU I) funded by Ministry of Education Youth and Sports of Czech Republic.

References
DETERMINATION OF TRACE CONCENTRATIONS OF CHLORIDES BY CONTINUUM SOURCE HIGH RESOLUTION GRAPHITE FURNACE ATOMIC ABSORPTION SPECTROMETRY

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Trace concentrations of chlorides in aquatic samples were determined by graphite furnace continuum source high resolution atomic absorption spectrometry (GF-CS-HR-AAS) by making use of formation of diatomic InCl species. The influence of indium concentration, chemical modifiers, ashing and atomisation temperatures was investigated.

The detection limit and precision of the method are below 1 µg/l and 5 %, respectively. The method was used for analysis of various water samples including surface water, underground water and wastewater.

Keywords: chloride, CS HR AAS

Acknowledgments
The financial support by the Competence Center for SMART Technologies for Electronics and Informatics Systems and Services, ITMS 26240220072, and the grant agency APVV (project No. APVV-0797-11) is highly appreciated.
During the operation of nuclear power plants, a significant amount of waste liquid is produced. This is commonly called run-off water/liquid, which contains a high concentration of boric acid from the primary circuit, as well as waste products from the decontamination and the regeneration of the primary water treatment plant. Because of the varying contributions from possible sources, this liquid has a complex matrix. The aim of the present work was to develop field-applicable LIBS methods for the analysis of Th, U and Cs in nuclear run-off water. The direct analysis of liquid samples by LIBS is hampered by several technical difficulties – in order to circumvent these, we also investigated the usefulness of various sample preparation and sample presentation methods.

For the sake of the improvement of the limits of detection, our sample preparation approach was to use extraction chromatography resins. We investigated the use of the CS, TEVA and UTEVA resins by Triskem for the separation and retention of cesium, thorium and uranium ions from the run-off aqueous matrix. The Cs (AMP-PAN) resin is based on a selective inorganic material (ammonium phosphomolybdate) which is embedded in an organic matrix (polyacrylnitrile). In case of the TEVA resin the selectivity is based on a quaternary ammonium salt (Aliquat® 336). The UTEVA resin has a polymer backbone which is coated with dipentyl pentylyphosphonate. The selectivity and the enrichment provided by the resins in this matrix were assessed by using ICP-MS spectrometry.

We also developed novel sample presentation methods for the LIBS analysis. The use of liquid to solid conversion sample presentation methods were investigated in in-house designed closed sample chambers. The methods investigated included: i) soaking up the liquid by a filter membrane which was then dried, ii) dropping and drying the liquid onto a prepared solid surface and iii) direct analysis of the loaded resin particles. The aliquot quantities analyzed were within the µL - mL range. The detection limits achieved based on the enrichment provided by the resins were in the range of 2-10 ppm.

In summary, fast, field-applicable methods for the analysis of U, Th and Cs in nuclear run-off water samples were successfully developed. The methods can be executed on a small volume of the sample.
SELF-ALIQUOTING MICRO-ARRAY PLATES IN COMBINATION WITH DRIED-DROPLET LASER ABLATION FOR THE QUANTIFICATION OF TRACE ELEMENTS IN WHOLE BLOOD

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When using inductively-coupled plasma mass spectrometry (ICP-MS) in order to determine the elemental composition of whole blood, usually, a chemical digestion is mandatory. By digesting the whole blood with, e.g., a combination of inorganic acids and oxidizers at elevated temperature, organic constituents of the blood are broken down and, ideally, a purely inorganic solution is obtained. This facilitates quantification, as the matrix of a digested sample approaches that of an inorganic calibration standard. Moreover, the sample is diluted which minimizes the likelihood of nebulizer blockage.

However, digestion of whole blood is a tedious procedure and can result in contamination or losses of analytes. Moreover, digestion is time-consuming, making it hard to obtain information in a timely manner.

In this contribution, we present a rapid procedure for trace-elemental screening of whole blood. The method of choice is dried-droplet laser ablation in combination with ICP-MS. Previously, we presented a method using pre-cut filter disks and a radial ablation pattern for the analysis of samples with a matrix composition quite similar to whole blood [1] which was based on the approach presented in [2]. Here, we take the method one step further by using self- aliquoting micro-array plates, by adapting a sample-preparation technique originally designed for MALDI-MS measurements [3]. This allows to automatically split one blood sample into reproducible aliquots, thus avoiding manual pipetting and improves statistics by increasing the number of replicates without increasing the time required for sample preparation.

We will present the capabilities of the method in terms of sensitivity, reproducibility, and accuracy by analyzing Recipe ClinChek® Whole Blood Controls levels I, II, and III.

References
ANALYSIS OF TOXIC TRACE METALS IN ULTRAFINE AIRBORNE PARTICULATES USING LA-ICP-MS

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Numerous epidemiological and toxicological studies have found associations between measured particulate matter (PM) levels and adverse health effects. A PM fraction that is known to exert toxic effects is the metallic portion. Therefore, the concentrations of several toxic elements are routinely monitored in several countries. For this purpose, usually the size fractions below 10 µm and 2.5 µm aerodynamic diameter (PM₁₀ and PM₂.₅ respectively) are considered. However, for ultrafine particles (UFP) an enhanced toxicity is expected since the respiratory deposition is distinctly increased when compared to larger particles, which were separated to a bigger part in the in the pharyngeal and tracheal region. Information about the occurrence of trace metals in UFP is rather sparse, problems in analysis due to complex composition of PM and restricted sample amounts are the main limitations.

In this contribution an LA-ICP-MS procedure is presented, which allows quantitative analysis of transition metals in size segregated PM samples. Collection of UFP has been performed using a low pressure impactor. Particles ranging from 0.03 to 10 µm were deposited on high-purity polycarbonate as sampling substrate. For analysis from each impactor stage a representative number of sample spots has been analyzed. Complete ablation of sample spots was enabled with the use of line scan patterns adjusted to the size of the respective sample spots (ranging from less than 100 to several 100 µm diameter). Quantification of derived transient signals was accomplished with dried micro-droplets prepared using self- aliquoting micro-array plates. With this approach, the applied aqueous standard solutions were automatically split into reproducible aliquots, which are distributed in a well-defined grid pattern across the surface, simplifying localization and measurement of the residues after solvent evaporation.

The developed LA-ICP-MS procedure has been applied for the analysis of UFP samples collected in the urban area of Como, Italy. Accuracy of results has been demonstrated by conventional ICP-MS analysis of selected UFP samples after complete sample mineralization with mineral acids.
CALIBRATION APPROACHES IN LASER ABLATION INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (LA-ICP-MS)

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Micro – destructive character and lack of complex sample preparation step, including digestion, made mass spectrometry with laser micro-sampling one of the fastest developing technique of solid samples analysis. Laser ablation (LA) coupled to mass spectrometry (ICP-MS) allows simultaneous determination of many elements, yet it requires setting the calibration dependency between signals and concentrations. Analytical signals are influenced by sampled mass, dependant on the sample – laser beam interaction, matrix components, atomization, ionization, transport and finally analysis of ablated material. Construction of such physicochemical model which considers all of the mentioned factors, would allow quantification on the base of calibration with non matrix – matched standards. This task is however difficult and taken only in a narrow extent, e.g. through introduction of, usually empirical, correction coefficients. Hence, for calibration of LA-ICP-MS analyses, mostly solid standards with matched matrices are applied. Commercially available standards are usually in a form of glasses which not cover matrices of materials to be in analytical consideration.

Among calibration methods used in LA-ICP-MS analyses [1,2] three approaches can be distinguished, based on exploitation of: reference materials of matched matrices, reference materials adjusted in terms of analytes concentrations, and liquid standards introduced into plasma simultaneously with ablated portion of a sample. In all approaches, measurement of internal standard signal is recommended. It allows minimizing the influence of standards inhomogeneity and sampling differences or fractionation effects.

The presentation will involve discussion of different factors influencing analytical signals in LA-ICP-MS and calibration procedures. Additionally, selected techniques of signals standardisations will be also considered.

References

Session 3 - Laser spectroscopy II ESAS-2016-OL-10
Laser ablation was performed by nanosecond excimer laser ablation system. Different materials and different ablation conditions were used for the study of the aerosol formed during laser beam-sample interaction and for the study of the ablation craters.

The particle size distribution (PSD) of dry aerosol was monitored simultaneously with LA-ICP-MS (Laser Ablation Inductively Coupled Plasma Mass Spectrometry) analysis using two aerosol spectrometers – Fast Mobility Particle Sizer (FMPS) and Scanning Mobility Particle Sizer (SMPS). The unique combination of LA-ICP-MS and FMPS offers the possibility of controlling the particle size distribution every 1 s of the ablation process in the size range of 5.6 – 560 nm.

Ablation craters were additionally studied using scanning electron microscope, digital microscope and energy dispersive X-ray analysis. The link between laser ablation conditions, particle formation and elemental fractionation was discussed.

**Acknowledgements**

This work was supported by the European Regional Development Fund project “CEITEC” (CZ.1.05/1.1.00/02.0068). The authors would like to thank TESCAN Brno and Dr. Jozef Vincenc Oboóa for high resolution SEM micrographs. V.K. acknowledges Czech Science Foundation for a grant to support the project S 14-13600S. H.N. and V.K. acknowledge support of the project MUNI/A/1461/2014 from Masaryk University Specific Research Programme. J. O. acknowledges Czech Science Foundation for a grant P503/12/G147. This work was also funded by the European Social Fund, project “Support of inter-sectoral mobility and quality enhancement of research teams at the Czech Technical University in Prague” (CZ.1.07/2.3.00/30.0034).
Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) represents one of the most suitable method for study of lateral distribution of specific elements (Cu, Zn, Pb, Pt...) in low concentration levels (tens mg/kg) in various biological tissues.

Presented work is focused on study of influence of scan speed and laser spot diameter on lateral resolution, LOD, and time consumption of analysis. The utilization of LA-ICP-MS for bioimaging purpose will be demonstrated on two different types of the matrices. First one is tumour tissue which is treated by various Pt-based cytostatics (carbo-, oxali- and cis-Pt). The second one are cuts of tapeworm treated by various heavy metals.

This project was supported by Czech Science Foundation GA13-18154S, by the project “CEITEC - Central European Institute of Technology” (CZ.1.05/1.1.00/02.0068) from European Regional Development Fund.
The determination of elemental impurities, undesirable components without therapeutic benefit, in pharmaceutical product has recently gained interest in quality control laboratories of pharmaceutical production. The elemental impurities, particularly heavy metals may be introduced into the drugs from different sources. Consequently, their levels should be strictly controlled in drug products due to their adverse effect on human health [1].

In this contribution we will reflect current changes in guidelines concerning to the establishment of the permitted daily exposure value (PDE) for different administration route, safety assessment as well as the development of reliable analytical procedures (ICP-OES/MS). Namely ICH Q3D [1] and United States Pharmacopeia (USP)'s general chapters for elemental impurities ( <232> Elemental Impurities – Limits and <233> Elemental Impurities – Procedures) will be discussed [2,3].

Requirements, that laboratory interested in analysis of metal impurities for pharmaceutical industry, have to fulfil will be mentioned. Furthermore some experience with implementation of these requirements in R&D lab will be presented. This task covers instrument qualification, method validation, and preparation of Standard Operation Procedures. Finally, real samples can be analysed which involves sample preparation that can bring some more difficulties [4].

References
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Acknowledgements
The authors gratefully acknowledge the support from the Ministry of Education, Youth and Sports of the Czech Republic LO 1305.
MICROBIAL CHARACTERIZATION OF OUTDOOR SAMPLES IN SMOKE AND NON-SMOKE AREAS USING VITEK-MS AND THEIR EFFECT ON HUMAN HEALTH

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Istanbul is one of the most crowded cities in the world. This population density has a constant negative effect for human health, nature and ecology. The most important negative effect is caused by the air quality and contents. Air quality is defined by atmospheric particulates which evolved by different chemical and physical mechanisms and spread to atmosphere with combustions happening in industrial processes or some other natural processes. These particulates participate in many different chemical processes at atmosphere and directly or indirectly take part producing clouds to decrease visibility, increasing acid deposition and changing atmospheric radiation balance. Concentration and composition of these particulates constantly changing with their size, location and exposure time which are mainly effected by convective and diffusive transfers, effectiveness of removal mechanisms and meteorological parameters, like wind, rain etc. Atmospheric particulates evolved with these interactions have a huge microbiologic and chemically impact on air quality [1-3].

The outdoor atmosphere is an environmental unit that impacts on public health. To investigate the composition of organisms in air particulates, we optimized sampling strategies (culture media type, sample collection type, etc.) for the detection using automated system which is MALDI-TOF. After optimization of sample preparation of collected samples, microbial characterization was done by VITEK-MS, which is an advanced mass spectrometer for qualitative and quantitative analysis for bacteria and yeasts.

A comprehensive microbial characterization of urban aerosol collected with manual aerosol samplers in Istanbul (Turkey) was carried out during three months in 2015. Microbial species and meteorological data (wind, temperature, humidity, etc.) were compared and evaluated statistically.

References
Plants are complex organisms which account for 99% of the biomass on Earth. They are the first link of the food chain, located at the interface of soil, atmosphere and consumer. From the point of view of chemical composition, plants are approximately constituted of water and organic matter for 90% and approximately 10% of mineral elements in variable quantities which can be associated to a deficiency or an excess. Plants take up and store all the elements present in their environment. Several metal ions play an essential role (Ca, K, Mg, Fe,...) for vital specific functions. Inversely, some elements (Cd, Hg, Pb,...) can become rapidly toxic and are the subject of a constant attention. The significant role of element in plants is, then, an important field of research in physiology, nutrition and environment. However, the improvement of knowledge on their biochemical functions involves the use of analytical chemistry and, particularly, atomic spectrometry.

The principles of plant analysis were developed at the beginning of the 19th century (De Saussure). Since 1915 (Lundegardh), the digestion of plant samples, followed by the determination of the total contents by atomic spectrometry represents the traditional way of analysis. Today, the importance of metals in the biological systems and the improvement in instrumentation technology (ICP-MS) led to the emergence of new analytical challenges. The aim of this communication is to show how the developments of the atomic spectrometry has played, and play as ever, an essential part in the plant science. After a short history, some recent applications and some future prospects are presented such as direct analysis of plants at the solid state, speciation, ionomic or the use of isotopic ratios.

Keywords: atomic spectrometry, plant samples
NEW PLASMA OBSERVATION APPROACHES FOR THE ANALYSIS OF PRECIOUS METALS

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ICP-OES with axial plasma observation are still the instruments of choice for trace analytical work. Even today, ICP-OES still plays an important role as it offers a much higher matrix tolerance than other techniques and is therefore beneficial for certain types of samples and/or elements.

Viewing the plasma radially provides generally lower sensitivity, but matrix effects are greatly reduced. Therefore the radial observation technique is typically chosen in the case of samples with high TSD (total dissolved solids) concentrations, for the routine analysis of organic solutions or where high stability and precision is required.

The possibility to view the plasma with two interfaces (dual view) seems to solve all disadvantages, but those techniques are a compromise since only one light path is direct.

For the analysis of precious metals high precision and accuracy for the main components is required. At the same time the wish for low detection limits for the trace elements in the matrix makes the task more challenging.

In the presentation new techniques to solve this dilemma will be discussed.
SIMPLE MEANS TO ENHANCE ROBUSTNESS IN AXIAL VIEW USN-ICP OES VIA AN ADDITIONAL NITROGEN GAS STREAM

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In the present study a low flow of N₂ is mixed with the aerosol exiting an ultrasonic nebulizer (USN) prior analysis using inductively coupled plasma optical emission spectrometry (ICP OES). The foreign gas is added via a plastic mixing tee for improving plasma characteristics in axially-viewed argon ICP. By computing the Mg ionic to atomic ratio (plasma robustness) using a conventional pneumatic nebulizer (PN) and USN, it was concluded that N₂ dissociates closer to the load coil when USN is used, i.e., partially dried plasma conditions. The maximum emission intensity of Mg(II) for PN was observed at 11 mm from the load coil while it was 8 mm for USN, indicating earlier aerosol desolvation, atomization and excitation processes in the ICP. Emission profiles of Ar(I) 415.861 nm, Ba(II) 486.601 nm and Ba(II) 233.527 nm indicated that metastable Ar species are overpopulated in the ICP under the N₂ flow and the electron impact excitation path present a smaller magnitude in the central channel. Copper and manganese ionic lines with energy close to 16 eV (Ar ionization) were monitored to evaluate spatially dependent charge-transfer reaction along the ICP axis in the presence and absence of the N₂ flow. Profiles of Cu(II) indicated abundance of Ar⁺ species at low distances from the load coil when N₂ was added. [1] On the other hand, differences were not observed at longer distances from the load coil for both plasmas (mixed-gas and pure Ar-ICP). Radial Cu(II) profiles have also shown a low N₂ diffusion until 3 mm from the ICP axis. The calculated limits of detection (LODs) for both plasmas had the same order of magnitude. Analysis of certified reference samples demonstrated that the accuracy was preserved by adding the low flow of N₂. It was concluded that adding a low flow of N₂ to the aerosol produced by USN via a tee is a simple way to increase plasma robustness, which is usually lower due to partially dried plasma conditions than that achieved using conventional PN.

**References**

GOLD NANOPARTICLE CHARACTERIZATION USING LASER-ASSISTED SAMPLE INTRODUCTION TO ICP MS

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Nanomaterials have entered virtually all areas of everyday life: from cosmetics and medicine to energy production and waste management. A range of tools has been proposed for characterization of nanomaterials; one of the established methods is inductively coupled plasma mass spectrometry (ICP MS) operated in the single particle mode. For this purpose, nanoparticles (NPs) are introduced to plasma torch using nebulizers or microdroplet generators.

We describe new laser-assisted approaches of nanoparticle introduction to ICP MS from solid surfaces: substrate-assisted laser desorption (SALD) and diode laser thermal vaporization (DLTV). Both techniques were originally employed for introduction of liquid samples in sub-microliter volumes into ICP. In SALD, samples are deposited and dried on a strongly absorbing plate which is ablated with a frequency-quintupled Nd:YAG laser (213 nm) operated at rather low fluence. We demonstrate that individual intact NPs can be efficiently desorbed from the surface and carried to a plasma torch. Experimental conditions, such as the laser fluence, sample scan rate, carrier gas type and flow rate were carefully optimized in order to gain highest NP signal and transport efficiency and to reduce NP disintegration within the desorption step. SALD ICP MS was validated using well characterized, commercially available Au NPs. The results are compared with a routine nebulizer ICP MS and applicability of the technique for NP characterization is discussed.

In addition, we also present initial NP analyses using DLTV. In this case, NPs are deposited on black rectangles printed on paper strips and released by thermal decomposition of paper using a continuous near infrared laser (808 nm).

Acknowledgments
We gratefully acknowledge the financial support from the projects GA15-05387S and CEITEC 2020 (LQ1601).
Optimization of ICP-MS Instrumental Parameters for Single Nanoparticle Analysis

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Engineered nanoparticles (NPs) are more and more used in consumer products, thus the development of fast and practical analytical methods for their characterization are needed. A promising novel characterization method is Single Particle Inductively Coupled Plasma Mass Spectroscopy (SP-ICP-MS), which shows distinct advantages over other characterization methods in the case of NPs dispersed in water. The particle size detection limit is around 15-30 nm, and concentrations above $10^3$/mL can be measured in about 5 minutes. The usefulness of SP-ICP-MS has already been demonstrated in a few environmental, biological and food chemistry applications.

It has already been established in the literature that the NP concentration, dwell time and acquisition time have to be optimized concertedly for a successful SP-ICP-MS measurement. The influence of further instrumental parameters, such as the plasma RF power, sampling depth and aerosol dilution gas flow rate have not yet been studied earlier in SP-ICP-MS, although they are known to have a great influence on the analytical performance in solution ICP-MS. For the first time in the literature, we carried out systematic experiments in the present study to reveal the impact of these parameters on the SP-ICP-MS analytical figures of merit. Standard gold and silver nano dispersions were used as samples. In addition, we also studied the possibility of using the He collision cell technology (CCT), now standard on all ICP-MS instruments, for the elimination of spectral interferences that hamper the measurement of certain NPs. In these experiments, hematite, ZnO and Cr₂O₃ nanoparticles were used. All experiments were carried out on an Agilent 7700x ICP-MS instrument.

Our results show that helium collision cell technology can be advantageously used for the elimination of spectral interferences without compromising the statistical quality of the NP data. Size detection limits also did not change significantly when CCT was used. It was found that the optimization of the sampling depth and plasma RF power can provide a several-fold increase in sensitivity, also depending on the mass of the monitored isotope. At the same time, it was revealed that the control of the aerosol dilution gas flow rate, which is a useful tool in solution analysis for the dilution of the matrix, is not efficient for the on-line dilution of NP dispersions.
THE EASY WAY OF ANALYSING OIL SAMPLES USING ICP-OES SPECTROMETRY IN RADIAL VIEW

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The quantitative determination of elements in oil samples is a typical application for simultaneous ICP-OES spectrometers. There is a wide variety of samples from different market segments such as petrochemistry, automotive, food and more. In the petrochemical field, ICP-OES is used for a broad range of analysis in order to manage trace amounts of hazardous metals in the manufacturing process, manage additive elements essential to the functionality of a product, and manage the environment of the entire factory. In the automotive industry the interest is for (bio-) fuels, lubricants, additives and more. Last not least there are a lot of food samples such as edible oils which needs to be determined according to their composition of major-, minor-, and trace elements.

Therefore, it is desirable to have a robust, highly stable system able to reliably accept the injection of a broad variety of samples, regardless of the type of solvent (aqueous/organic) or the presence of matrices. It is also important to simplify processes and reduce costs, which enhances the productivity of daily quality control work. When the ICPE-9820 is used to analyze high-concentration samples or inject certain organic solvents (such as xylene), the cooling jacket can be removed to use the unit exclusively for the radial view.

This easy way of direct sample injection has been done on a variety of oils with different levels of element concentrations. The analytical data will be presented and advantages of this method will be discussed.
LA-ICP-MS IMAGING DATA AS A SUPPORT FOR PIGMENT IDENTIFICATION

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The usefulness of incorporation of LA-ICP-MS to the process of historic pigments’ identification was evaluated to be beneficial while only minute amounts of particles can be taken from unique and valuable objects. The dimensions of all taken micro-samples were strictly controlled not to exceed hundreds of micrometers and not to affect the visible stage of the investigated objects from the Museum. These particles were subjected to a sequential use of selected instrumental methods to collect elemental and molecular information by means of:

(i) Field Emission Scanning Electron Microscopy equipped with Energy Dispersive Spectroscopy (FE-SEM EDS, Zeiss Merlin with Bruker Quantax 400);
(ii) Raman spectroscopy (Labram HR800, Horiba Jobin Yvon and Nicolet NXR FT-Raman Spectrometers) and
(iii) Laser Ablation Inductively Coupled Plasma Mass Spectrometry (ELAN 9000, Perkin Elmer with SCIEX LSX-213, CETAC).

The coherency of all obtained results was evaluated for each sample before the final interpretation according to one out of the three possible scenarios relying either on (1) the results of major elemental information obtained by SEM-EDS and molecular information obtained by Raman investigations, which were clear, coherent and sufficient to propose the basic pigments identification or (2) the results of major elemental information obtained by SEM-EDS supported by LA-ICP-MS measurements of the samples and molecular information obtained by Raman investigations, which were coherent and sufficient to propose the pigments identification. The identification of 3 out of 30 samples were assumed only on the basis of their elemental composition and chemical similarity to the others proposed in accordance to (3) the general elemental information obtained by SEM-EDS and LA-ICP-MS. For these samples Raman spectra were strongly affected by fluorescence and the selection of the suitable excitation wavelength (532, 785 or 1064 nm) was not possible.

For all micro-samples LA-ICP-MS imaging data were collected to evaluate the particles homogeneity, however for the last group of pigments these results were of the highest importance for the final interpretation and will be discussed with details.
SHIMADZU’S CORPORATE PROFILE; 140 YEARS OF EXCELLENCE IN SCIENCE

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Since its foundation in Kyoto, Japan, in 1875, Shimadzu has grown from a 1 man company to a multinational market leader with almost 11,000 Employees divided over 4 major business units.

Many highlights, including a Nobel Prize in 2003, grace the companies 140 year history. The main driving force behind Shimadzu’s organic growth has always been; Contributing to society through Science & Technology.

This presentation will give you a bird’s eye view on Shimadzu’s organizational structure, product portfolio and local presence in your area.
Microwave Plasma - Atomic Emission Spectroscopy (MP-AES) represents a completely new elemental analysis technique that has been designed to improve analytical performance and productivity, while decreasing operating costs by eliminating the flammable and/or expensive gas requirements used in typical elemental analysis techniques. The Nitrogen based plasma operates from a compressed air supply and Nitrogen generator, resulting in a significant reduction in operating costs and reduced infra structure costs. In addition, the state-of-the-art design of the Agilent 4200 MP-AES reduces the number of costly consumables such as hollow cathode lamps used in Atomic Absorption techniques.

The MP-AES technique produces superior linear dynamic range, detection limits and analysis speed compared to conventional flame Atomic Absorption Spectroscopy. Based on an atomic emission technique, this elemental analysis technique produces simpler spectra than ICP-OES and greater sensitivity than flame AAS.

We present an overview of the MP-AES technique, hardware, software and its capabilities. Performance is demonstrated for a range of sample types including examples from the geochemical, petrochemical, agricultural and environmental areas.
INSIGHTS INTO THE CHEMICAL VAPOR GENERATION OF CADMIUM AT TRACE LEVEL

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Chemical vapor generation (CVG) of cadmium by aqueous boranes has been investigated by using continuous flow reaction system coupled with quartz tube, diffusion miniature flame atomizer and atomic absorption spectrometry, with the aim to clarify some of the mechanisms controlling the generation of volatile species. Experimental evidence that BH₃OH⁻ is the most likely effective species in the generation of volatile Cd species. It can be synthesized on-line by quenching the acid hydrolysis of BH₄⁻ by NaOH, according the following reactions [1]:

\[ \text{BH}_4^- + \text{H}_3\text{O}^+ \rightarrow \text{BH}_3(\text{H}_2\text{O}) + \text{H}_2 \]
\[ \text{BH}_3(\text{H}_2\text{O}) + \text{OH}^- \rightarrow \text{BH}_3\text{OH}^- + \text{H}_2\text{O} \]

The use of BH₃OH⁻ in alkaline conditions increases sensitivity of about a factor 2.2 with respect to BH₄⁻, indicating an improved generation efficiency.

A further parameter controlling dramatically the sensitivity was the presence of dissolved oxygen in the reagents. Removal of oxygen from analyte and reductant solutions, by argon purging, resulted in a sensitivity improvement of about 8 fold and 6 fold by using BH₄⁻ and BH₃OH⁻ reductant, respectively. Oxygen gas added between gas-liquid separator and the atomizer hardly affects the sensitivity, indicating that the oxygen interferes mainly in the liquid phase, during the generation step of volatile Cd species. The oxygen effect is dramatically dependent on Cd(II) concentration in the range from about 0.5 to 150 ng Cd/mL. Interference effects from Cu(II), Fe, Ni and Co are severe and can be related to the strongest hydride character of BH₃OH⁻ with respect to BH₄⁻.

References
ON THE POSSIBILITY OF THE DETERMINATION OF DEUTERIUM BY ICP-MS

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The determination of the deuterium content of solvents and other liquid samples is of high importance in several fields of science and industry. This analysis is nowadays typically performed by infrared spectroscopy, laser absorption spectroscopy or by special mass spectrometry instrumentation (such as accelerated MS or low mass multicollector MS). At the same time, ICP-MS analysis of deuterium is not described in the literature – partially due to the fact that many ICP-MS instruments are not built to operate in the lower extreme end of the mass range needed for direct deuterium analysis.

In the present study, we carried out a detailed assessment of the possibility of the determination of the deuterium content of aqueous samples by using a standard quadrupole Agilent 7700x ICP-MS. Several direct and indirect analysis options (the latter via the measurement of hydrogen-containing polyatomic adducts) were investigated. The influence of instrumental parameters on the monitored signals was systematically studied. Signal repeatability and stability, memory effects, as well as hot and cool plasma conditions were also tested. The standard I-AS automatic sample introduction system with a Peltier-cooled Scott-type spray chamber and a Mira Mist nebulizer were used in the tests. Certified deuterated and deuterium-depleted reference samples (NMR solvents by Sigma Aldrich) were used as model solutions.

It was established that under optimized conditions, quadrupole ICP-MS deuterium analysis is indeed a feasible and practical option. The analysis is characterizable with ppm-range detection limits, a 3-4 orders of magnitude linear dynamic range and a 1-5% relative error.
The objective of this work was to determine the contents of selected toxic and essential ultra-trace elements in fruits of service tree (Sorbus domestica L.) depending on maturity state. These elements were furthermore quantified in the leaves and bark of the trees in order to investigate their accumulation pattern. All samples were dried and digested using an acidic microwave assisted digestion system prior to quantification by inductively coupled plasma – mass spectrometry. The elements chosen were Arsenic and Cadmium as well as Lithium, Molybdenum, and Selenium. The Arsenic content rose with maturity in peel as well as mesocarp. Cadmium found in the mesocarp was unaffected by ripeness, its content in the peel was below the limit of detection of all three ripeness states. For Lithium and Molybdenum no statistical significant effect of ripeness could be found on their content neither in peel nor in mesocarp. Selenium could not be detected in the majority of fruit samples, thus no conclusion could be drawn on the dependency on ripeness.
Beer is the most popular alcoholic beverage in Europe. In Germany, beer enjoys a particularly high status due to the German Beer Purity Law of 1516 (the “Reinheitsgebot”), which uniquely defines the ingredients of beer to be hops, malt, yeast and water. This makes the German Beer Purity Law the oldest food law in the world, which is still valid today and makes beer, in addition to drinking water, one of the most researched food products with the highest standards regarding quality, freshness, appearance and flavor. Statistically, per capita beer consumption in European countries was 68 liters in 2013. The highest per capita beer consumption was determined for the Czech Republic (144 L), followed by Germany (107 L) and Austria (106 L). For these levels of consumption, the question arises: just how healthy is beer and what does beer contain?

In accordance with the German Beer Purity Law of 1516, German beer contains the ingredients hops, malt, yeast and water, as well as all major B vitamins. Vitamin B2 and B6, which are important for metabolism, are particularly abundant in beer. In addition, bitter substances and essential oils are indisputably effective against loss of appetite, gastric disorders and states of anxiety. Japanese scientists have found active ingredients in 24 types of beer that inhibit so-called heterocyclic amines and thus the onset of cancer. This has been confirmed by German scientists, who see the same tumor-preventing effects of the polyphenolic flavonoids as are claimed for red wine. Last but not least, beer is diuretic, and its phenolic ingredients support the cardiovascular system. In addition, beer contains minerals and trace elements (e.g. Ca, Na, Mg and Zn) that are important for human nutrition. However, undesirable substances such as heavy metals (for instance Cd, Pb, Hg and As) are also found.

For simultaneous multi-element analysis, an atomic emission spectrometer with an inductively-coupled plasma like the ICPE-9820 with vertical minitorch position and ‘dual view’ (axial and radial) plasma observation has been used. This method enables the analysis of samples with low concentrations of just a few µg/L (axial) such as Pb, Cd, Mn, Hg, As and Sb and high concentrations of approximately 0.5 mg/L up to 150 mg/L (radial) such as Na, K, Ca and Mg within a single analysis sequence. Implementation of this method is carried out in accordance with DIN EN ISO 11885 (2009). The beer samples were degassed for 5 minutes in an ultrasonic water bath and subsequently diluted with water to 1:1 and 1:5 respectively. Calibration was performed against aqueous standard solutions. Analytical results for a variety of beers are presented.
DETERMINATION OF TRACE ELEMENTS IN THE OPEN OCEAN: METHOD VALIDATION

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Oceanographic research over the past few decades has unveiled the significance of trace metals in marine biogeochemical cycles. Trace element determination in seawater is analytically difficult, due to the typically very low concentrations and the potential interference of the salt matrix. Determination of trace elements contents in the low ng kg⁻¹ level remains a fundamental analytical challenge and a great source of complexity also for the realisation of reliable profiles of dissolved trace elements in the ocean.

Although the detection sensitivity of ICP-MS allows the direct measurement of trace elements at sub-ng g⁻¹ levels the physical deposition of salts on interface cones and polyatomic interference from the major ions in seawater does not allow a simple analysis. Therefore, sample pre-treatment or matrix elimination prior to sample introduction into the plasma is often inevitable.

A method based on the application of an automated off-line seaFAST preconcentration system, combined with subsequent HR ICP-MS determination was developed. The column integrated into seaFAST contained chelating resin with ethylenediaminetriacetic acid and iminodiacetic acid functional groups. The nine trace elements (Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb) were simultaneously and quantitatively preconcentrated from 10 mL of seawater, eluted with 200 µL of 1.8 M HNO₃, and determined by HR-ICP-MS using external calibration method. The single-step preconcentration removed more than 99.9% of Na, K, Mg and Ca from seawater.

ISO-17025 and Eurachem guidelines were followed to perform the validation of the proposed methodology. Accordingly, blanks, selectivity, linearity of the calibration curve, working range, recovery, precision, traceability, limit of detection, limit of quantification and expanded uncertainty were assessed. The estimation of the total uncertainty associated to each measurement result was fundamental tool for sorting the main sources of measurement biases. Preliminary forecast of the uncertainty budgets was used as a strategy to ensure that determination of trace elements in sea water could be achieved with demonstrated traceability to a stated system of reference within less than 10 % expanded uncertainty (k=2) respectively.

Additional validation of the developed analytical procedure was effectuated by comparison with the results obtained with ET-AAS method and with the values reported in the frame of EC JRC IRMM certification exercise. ID ICP-MS applied as a primary method of measurements was used for cross validation of developed analytical procedure for selected trace elements.
CHARACTERIZATION OF STRUCTURAL POSITIONS OF IRON IN BIOLOGICAL TISSUES

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Iron is one of the most important nonorganic substances that make life possible [1]. It is required for active sites of many metalloproteins that play key role in crucial biological processes such as oxygen transport, storage, and use of oxygen in many oxidation-reduction reactions as well as in electron transfer reactions within the cell [2, 3]. Iron is also important for processes of synthesis such as DNA synthesis, heme and iron-sulfur cluster synthesis, etc [1]. Therefore it is necessary to know structural positions of iron in biological tissues in detail.

In the current work, we focus on characterization of iron in biological tissues. We studied three types of samples prepared from human brain, human and horse spleen. Mössbauer spectrometry measurements were performed at room (~300 K) and liquid helium (4.2 K) temperature. A conventional constant acceleration spectrometer with $^{57}$Co source in a rhodium matrix was used. The obtained Mössbauer parameters provide information on oxidation states, spin states, and the structure of iron in biological tissues. Low temperature measurements confirmed superparamagnetic behaviour of some spectral components. In addition to Mössbauer spectrometry also other methods such as neutron activation analysis and atomic absorption spectrometry were used for the sample characterization.

Acknowledgements
This work was supported by the projects VEGA 1/0220/12, VEGA 1/0836/15, SK-CZ-2013-0042 and by the Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies with the following logo

References
Effect of coating of eight different carboxylic acids (glycolic, propionic, lactic, malic, tartaric, citric, mandelic, caproic and caprylic) on nanostructured magnetite [1] was studied by Raman, photoacoustic and $^{57}$Fe Mössbauer spectroscopy. Raman spectroscopy indicated significant differences among the samples correspondingly to the reactions occurring with different acids. Accordingly, differences were also observed in the photoacoustic absorption spectra of samples coated with different carboxyl acids. Mössbauer spectroscopy of frozen solution samples showed dominantly magnetically split envelopes. The temperature dependent Mössbauer measurements clearly indicated the superparamagnetic nature of the nanomaterials at higher temperatures due to their small enough particle size in good correlation with the results of microscopy measurements. Mössbauer and Raman spectroscopy indicated a variation of relative intensity of components belonging to nanomagnetite and nanomaghemite. A correlation of the change of nanomaghemite microenvironments on expense of nanomagnetite ones with the acidity of carboxylic acids will be discussed.

Acknowledgements
The financial supports from the CAPES (No A127/2013) and OTKA (No K115913 and K115784) grants are acknowledged.

References
Iron oxides are wide-spread in nature and form stable compounds, which can be relatively easily synthesized in a laboratory. There are presented in every component of environment (atmosphere, biosphere, hydrosphere, litosphere, pedosphere …) [1]. Study of these oxides is especially important in material research, because they appear as corrosion products in construction materials and steels [2]. Mössbauer spectrometry (MS) is particularly suited method for characterization of iron properties in steel materials. This technique can determine iron oxidation state as well as arrangement of iron lattice (bcc – body-centred cubic, fcc – face-centred cubic).

In the current work, we focus on characterization of iron environments in LC200N steel by MS, neutron activation analysis (NAA), atomic absorption spectrometry (AAS) and X-ray fluorescence (XRF). We have investigated samples of steel with different thermal history. Namely, hardened, annealed, and annealed with rapid quenching. The element characterization was determined by NAA and XRF. Differences in chemical compositions were revealed in the as-cut and polished samples. By parameters of the Mössbauer spectra we were able to identify variations in the microstructure imposed by different numbers of admixture atoms in the first neighbourhood of central resonant iron atoms in the lattice.

Acknowledgements
This work was supported by the projects GACR 14-12449S and VEGA 1/0203/14 and by the Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies with the following logo

References
MÖSSBAUER SPECTROSCOPIC STUDY OF THE OXIDATION STATE OF IRON IN PLANT ROOTS DURING THE IRON UPTAKE PROCESS

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Despite being the fourth most abundant element in the earth’s crust, Fe is not readily available for plants due to the low solubility of iron oxides/oxyhydroxides at the pH of many soils. The low bioavailability of iron causes a common nutritional disorder that alters plant morphology and physiology even prompting plant death. To cope with this problem, Fe can be supplied as synthetic or natural Fe complexes applied in soils. However, it is rather difficult to predict the effectiveness of such Fe-complexes. For this reason, the knowledge on Fe speciation, redox transitions in the presence of plant-associated compounds, are of great importance.

In the present work, Fe compounds formed in roots of plants having different iron uptake mechanisms were investigated by Mössbauer spectroscopy, when a divalent $^{57}$Fe-complex, $^{57}$Fe(II)-ascorbate, was applied as iron source.

Typical Mössbauer spectrum of iron deficient roots supplied with $^{57}$Fe²⁺-ascorbate shows the presence of both Fe³⁺ and Fe²⁺ species. The iron(III) components were identified as mainly high spin Fe³⁺-carboxylate complexes probably attached to the cell wall while Fe²⁺ can be attributed to high spin Fe²⁺-hexaaqua complex. The relative amount of the Fe³⁺ depends on both the concentration and the duration of iron supply. Moreover, the ratio of Fe²⁺/Fe³⁺, thus the oxidation rate of Fe²⁺ to Fe³⁺ during the Fe uptake process was shown to be different in plants having different iron uptake mechanisms.

The results obtained can help to follow the oxidation after the Fe²⁺ uptake, and thus, to help understanding the redox transformations in the case of the known iron uptake mechanisms.

Acknowledgments
This work was supported by Hungarian National Science Fund grants National Research, Development and Innovation Office – NKFIH PD 111979.
Deep geological disposal of high-level radioactive waste (HLW) into argillaceous rock formation is foreseen as the potential radioactive waste disposal concept since it provides an effective physical and chemical barrier to restrain the migration of dissolved radionuclides. Several of the safety approaches for the geological disposal of HLW rely on the strong uptake of radio-contaminants by clay minerals. In Hungary, Boda Claystone Formation (BCF) is considered as the potential host rock formation for HLW disposal.

Micro- and macrospectrometric analyses were necessary to determine the sorption mechanisms between selected key cations and mineral phases occurring in the host rock. The main criteria among the selection of the cations were to provide most of all possible ions chemically representing radionuclides dissolved from HLW and if it is possible to deal with the non-radioactive form of the elements. Inactive Cs(I), Ni(II), Nd(III) and natural U(VI) ions were selected for the experiments. Thin sections were prepared from pre-characterized cores of BCF drillings on high-purity silicon wafers for microspectrometric investigations. They were reacted during 24-72-hour sorption experiments with the one ions of interest. The samples were measured with laboratory equipment and synchrotron radiation (SR) (microscopic X-ray fluorescence (µ-XRF), scanning electron microscopy energy dispersive X-ray analysis (SEM/EDX)) techniques. Laboratory µ-XRF is suitable to perform point measurements and to record two-dimensional elemental maps with 20–100 µm spatial resolution [1]. The evaluated elemental maps of Cs and Ni showed correlations between the Fe- and K-rich areas which are the main components of the argillaceous matrix. SEM/EDX was used to complete the µ-XRF results through investigating the low atomic number rock-forming elements in the loaded thin sections. For Nd and U the laboratory scale µ-XRF system is only a good pre-selection tool for SR measurements. SR µ-XRF measurements were performed on the same thin sections using 1-5 µm spatial resolution.

Multivariate data analysis was applied as a unique tool to obtain significant information from the µ-XRF and SEM/EDX elemental maps that can be related to the uptake of the element of interest by a particular mineral phase. In case of U and Nd the minerals responsible for the uptake were found to be not only the clayey matrix but the fracture infilling carbonate minerals also played an important role [2]. The uptake capacity of the different mineral phases could be quantified with additional mineralogical information [3].

The multivariate approach based on µ-XRF and SEM/EDX to identify the minerals was validated using microscopic X-ray diffraction.

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[1] Gergely F, Osán J, Szabó BK, Török S. Analytical performance of a versatile laboratory microscopic X-ray fluorescence (µ-XRF), scanning electron microscopy energy dispersive X-ray analysis (SEM/EDX)) techniques. Laboratory µ-XRF is suitable to perform point measurements and to record two-dimensional elemental maps with 20–100 µm spatial resolution [1]. The evaluated elemental maps of Cs and Ni showed correlations between the Fe- and K-rich areas which are the main components of the argillaceous matrix. SEM/EDX was used to complete the µ-XRF results through investigating the low atomic number rock-forming elements in the loaded thin sections. For Nd and U the laboratory scale µ-XRF system is only a good pre-selection tool for SR measurements. SR µ-XRF measurements were performed on the same thin sections using 1-5 µm spatial resolution.

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The multivariate approach based on µ-XRF and SEM/EDX to identify the minerals was validated using microscopic X-ray diffraction.

References
EXTENDING THE CAPABILITY OF PORTABLE XRF INTO NEW MARKETS AND APPLICATIONS

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For over twenty years, hand-held X-ray fluorescence (XRF) spectrometers have been used in scrap recycling and Positive Materials Identification in critical use applications such as refineries and chemical plants to verify correct alloy grade identification of simple metals.

With recent advances in instrument design including tube miniaturization, closer coupled optics and increased power, this has had an advantageous impact delivering improved limits of detection and quality of analysis.

This improved technology opens up new applications that typically have been the forte of laboratory testing but are now being replaced and/or complimented by portable XRF.

This presentation will outline the major performance improvements and how they are utilized in new vertical segments such as mining and consumer goods, and how they have extended the use of the analyzer into previously difficult materials such as carbon and low alloy steels.

In addition to performance improvement, the miniaturization has led to overall size and weight reductions extending operation in difficult to access locations.

With a “Smart and Connected” WiFi enabled analyzer, data and workflow management become possible and for large organizations fleet management becomes possible. This is the beginning of a new generation of analyzers.
SEQUENTIAL AND SIMULTANEOUS DETERMINATION OF Cd, Cr, Fe AND Al IN SOIL SAMPLES USING HR-CS GF AAS AND DIRECT SOLID SAMPLE ANALYSIS

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The proper use of soil amendments on a farm can significantly increase the quality of the harvested products. These procedures, however, may also result in soil contamination, mainly by potentially toxic elements. In this context, the soil analysis plays an important role to determine the presence of nutrients and contaminants in soil samples. The use of high-resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS GF AAS) with direct solid sample analysis may provide adequate information on the soil composition. This technique offers the advantage to perform to a certain extent multi-element analysis in sequential [1] and/or simultaneous [2] modes and even the possibility of determining additional elements via the absorption of diatomic molecules [3]. The aim of this study was the development of an analytical method for the sequential and simultaneous determination of Cd, Cr, Fe and Al in soil samples by HR-CS GF AAS, via direct solid sample analysis. The sequential mode allows the determination of Cd (228.802 nm) first, using 800 °C and 1700 °C as the pyrolysis and atomization temperature, respectively. After that, Cr (425.433 nm), Fe (425.076 nm) and Al (via the diatomic molecule AlH at 425.315 nm) can be determined simultaneously, using 2600 °C as atomization (Cr and Fe) and vaporization (AlH) temperature. Due to the high concentration of Cd present in the soil samples, an argon flow rate of 0.1 L min⁻¹ was applied in the atomization stage; moreover, secondary lines were used for Cr and Fe. The Al determination was carried out using the diatomic molecule AlH without the necessity to use a molecule-forming agent. However, aluminum is known to interfere in the determination of Cd; in order to minimize this interference 10 µL of 10% v/v H₂SO₄ was used in all measurements. Aqueous standard solutions were used for calibration and limits of detection (LOD) and quantification (LOQ) were obtained as 18 and 61 pg mg⁻¹ for Cd, 0.33 and 1.1 ng mg⁻¹ for Cr, 0.18 and 0.58 µg mg⁻¹ for Fe and 1.1 and 3.5 µg mg⁻¹ for Al. A certified reference material (CRM) of Montana Soil I (NIST – 2710a) was used to confirm the accuracy of the obtained results; the values found for all elements were in agreement with those reported for the CRM, proving that the developed method can be used to determine Cd, Cr, Fe and Al in soil samples.

Acknowledgments: CAPES and CNPq.

References
A STUDY OF CARBON-, SULFUR- AND PHOSPHORUS-BASED CHARGE TRANSFER REACTIONS IN INDUCTIVELY COUPLED PLASMA ATOMIC EMISSION SPECTROMETRY

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The influence of carbon, sulfur and phosphorus-based charge transfer reactions on the emission signals of Ag, Al, As, Au, B, Ba, Be, Ca, Cd, Co, Cr, Cu, Fe, Ga, Hg, In, Ir, K, Li, Mg, Mn, Na, Ni, P, Pb, Pd, Pt, S, Sb, Se, Sr, Te and Zn has been investigated in axially-viewed ICP-AES. The intensities of the atomic and ionic emission lines have been measured in diluted glycerol, sulfuric acid and phosphoric acid solutions and the results have been compared with the corresponding signals obtained for a 1% w w⁻¹ nitric acid solution. In the presence of carbon, sulfur or phosphorus signal enhancement has been observed for As, Se and Te atomic lines. The enhanced atomic emission intensities can be explained by a two-step mechanism: charge transfer from carbon, sulfur or phosphorus ions and, after an ion-electron recombination process, the population of excited analyte atoms is increased [1,2]. Iodine and P atomic emission intensities are enhanced by carbon and sulfur-based charge transfer whereas the Hg atomic emission signal is enhanced only by carbon. Although signal enhancement due to charge transfer reactions is also expected for ionic emission lines of the above listed elements, no experimental evidence has been found with the exception of Hg ionic lines operating carbon containing solutions. The effect of carbon, sulfur and phosphorus charge transfer reactions on atomic emission depends on: (i) wavelength characteristics. In general, signal enhancement is more significant for those electronic transitions involving the highest upper energy levels; (ii) plasma experimental conditions. The use of robust conditions (i.e. high r.f. power and lower nebulizer gas flow rates) improves carbon, sulfur and phosphorus ionization in the plasma and, hence, signal enhancement due to charge transfer is more pronounced; and (iii) the presence of other concomitants (e.g. K or Ca). Easily ionizable elements reduce ionization in the plasma and consequently decrease signal enhancement related to charge transfer reactions. Further research is required to explain why atomic emission signal enhancement is not registered for some elements (e.g. Au or Sb) despite they do have atomic energy levels that fulfill the requirements for charge transfer reactions and ICP-MS results suggest that they are involved in charge transfer processes [3,4].

References
DETERMINATION OF TRACE ELEMENTS IN FUELS BY MICROEMULSION BASED GFAAS METHOD

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Trace elements are released into the atmosphere by combustion of automobile fuel. Gasoline and diesel are used in huge amounts all around the world thus its trace element content can cause adverse health effects since some of the elements are very toxic or responsible for the depletion of antioxidants in the respiratory tract lung fluid. Furthermore, some metals catalyze oxidative reactions in hydrocarbon mixtures, degrading their thermal stability and may also cause corrosion and catalyst poisoning.

An easy, green and low-cost method was developed for the determination of copper in fuel samples by GF-AAS. The sample preparation method was based on a detergent free micro-emulsion prepared by mixing appropriate volumes of fuel, nitric acid, water and propan-2-ol. The volume ratios providing stable micro-emulsions were found experimentally. The efficiency of the mineralization with increasing amount of nitric acid was followed by standard addition of copper standards. Micro-volume spike was added to the micro-emulsion either as organometallic compound (cyclohexane butyrate, CHB) or aqueous standard to the organic and aqueous medium, respectively.

The efficiency of the mineralization with increasing amount of nitric acid was followed comparing the signals of aqueous spiked and CHB spiked samples and helped to choose the composition of the micro-emulsions. It was also proved that the (reaction) time between addition of the reagents plays no role in the mineralization. According to the pyrolysis curves of the aqueous spiked and CHB spiked micro-emulsions, no modifier was necessary for copper.

The samples can be analyzed by matrix matching calibration using aqueous standards and either commercial purified gasoline or laboratory-made acid-cleaned fuels. The copper recovery was between 95 and 115%. The detection limit (3s) for the whole analytical procedure was 0.36 µg/L in the original diesel sample. The dilution factor is 3.8 and 3.2 for diesel and gasoline, respectively. Good agreement was observed between the results obtained by this and comparative direct ICP-OES methods.

Change in the concentration of Cu in the micro-emulsion and the original diesel was also investigated during a 25 days long storage in plastic wares and no significant decrease was found.
APPLICATION OF ION-PAIRED REVERSED PHASE HPLC-ICP-MS FOR DETERMINATION OF EXTRACELLULAR SELENIUM SPECIATION IN SELENIUM-ENRICHED L. RHAMNOSUS CULTURE

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Determination of extracellular Se species in the remained-medium from the cultures of Se-enriched L. rhamnosus was carried out by HPLC-ICP-MS. The condition of HPLC-ICP-MS was for pH, 1-butanesulfonic acid and trifluoroacetic acid concentrations, type of separating column and flow rate, were 4.5, 8 mM, 4 mM, C18 (250 mm length × 4.6 mm I.D) and 1.2 mL min⁻¹, respectively. The remained-medium was separated from the biomass of Se-enriched L. rhamnosus which was cultured by supplementing SeO₃²⁻ ion into the MRS medium. It was prepared directly diluting with mobile phase solution and filtered with 0.45 nylon membrane prior to injecting into the HPLC-ICP-MS. It was found that SeO₃²⁻ ion and selenocysteine (Sec) was obtained as the major Se species in the remained-medium. The presence Sec and SeO₃²⁻ ion could be defined as free amino acid and non-transformed SeO₃²⁻ ion, respectively. The finding showed that SeO₃²⁻ ion is transported into L. rhamnosus cells, and synthesized to be Sec as a primary organic Se compound. The percentage recoveries of SeO₃²⁻ ion and Sec were 98 and 95 %, respectively. Therefore, the HPLC-ICP-MS was a key for determining the extracellular Se species of Se-enriched Lactobacillus culture which will extend the understanding of metabolism pathway of Se in Lactobacillus.

Keywords: HPLC-ICP-MS, Selenocysteine, Lactobacillus rhamnosus

Fig. 1 Chromatograms for recovery test; (a) RM from the culture of supplementing 2.5 mg Se L⁻¹, (b) spiked both standard solutions of SeO₃²⁻ ion and Sec.

References
STRATEGIES FOR IDENTIFICATION, QUANTIFICATION AND PRESERVATION OF ARSENIC SPECIES IN BIOLOGICAL SAMPLES

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The range of arsenic (As) concentration found in natural water is large, ranging from less than 0.5 µg/L to more than 5000 µg/L [1]. High-As groundwater areas have been detected in Hungary but aquifers found in Argentina, Chile, Mexico, China, West Bengal (India), Bangladesh and Vietnam are also affected by natural As contamination. In terms of population exposed to high As concentrations, the West Bengal basin leads with more than 40 million people. However, As toxicity depends on its oxidation state and chemical environment. Thus, inorganic As(V) and methylated As(V) species are less toxic than (in)organic As(III) species. Therefore, As speciation gives a more realistic information on the exposure to As than total As, although this latter is also necessary to be determined.

Conventional As speciation methods involve high performance liquid chromatographic (HPLC) separation on ion-exchange columns followed by hyphenation to an atomic spectrometric detector most commonly nowadays, inductively coupled plasma mass spectrometry (ICP-MS). For minute samples such as xylem saps, application of flow injection analysis (FIA) is also advisable for the total As determination. In terms of sample preparation, avoidance of interconversion of As species in the samples is mandatory. For example, about 5-10% of 150 µg/L As(III) in nutrient solutions is oxidized to As(V) in 48 h. For staple food items such as rice, enzymatic hydrolysis with α-amylase/protease and microprobe focused sonication is the most suitable procedure for fast extraction of As with high efficiency.

Development of alternative methods aiming at reducing the operational costs by substituting either HPLC or ICP-MS, or both has been attempted. Off-line hyphenation of (over-pressured)thin layer chromatography (TLC) with polyethylene imide cellulose plates to total reflection X-ray fluorescence spectrometry (TXRF) suffers from an acid microdigestion step of the developed TLC spots and reliable quantification for amounts greater than 25 ng of As(III), As(V), monomethyl arsonic acid and dimethylarsinic acid each. Replacement of this tedious sample preparation step by laser ablation – ICP –MS as well as application of non-chromatographic methods such as X-ray absorption near edge structure measurements with synchrotron-radiation-induced-TXRF analysis suggest that these methods may rather be of interest for qualitative monitoring of As species in biological samples. Solid phase extraction (SPE) with anion exchange cartridges proved to be reliable for on-site separation of inorganic As(III) and As(V) in drinking water in the low µg/L concentration. Then, the separated and acidified fractions can be easily analyzed by any appropriate atomic spectrometric techniques. However, FIA should be applied for elution from the SPE cartridges to quantify reliably all major As species in complex biological samples.

References
Antimony (Sb) is a cumulative toxic element for plants, animals and human health [1]. The Sb concentration of natural water is below 1 µg/L but it can reach 100 µg/L due to anthropogenic activities [2]. It has been extensively used for various industrial applications including batteries, semiconductors and fire proof textiles. The intake of excess of Sb from environment can cause diarrhea, skin rashes and respiratory problems even at trace levels [3]. Inorganic compounds of Sb are more toxic than its organic forms. The importance of determination of inorganic Sb in environmental samples is beside determination of total Sb.

The determination of inorganic Sb species by atomic spectroscopic techniques needs a sample preparation step before determination. Solid phase extraction is one of the important sample preparation steps for the speciation Sb. The speciation procedures based on solid phase extraction for antimony are generally based on the preconcentration-separation of one of the Sb species [Sb(III) or Sb(VI)]. In this procedure, total Sb was determined after the reduction of Sb(V) or by the oxidation of Sb(III)) according to bases of the procedure.

Speciation strategies investigated by our research group for inorganic Sb species based on solid phase extraction on Amberlite XAD-8, Chromosorb 102 resins, carbon nanotubes, silica, etc. are discussed in this presentation in order to determine Sb(III), Sb(V) and total Sb in natural water samples using flame or graphite furnace atomic absorption spectrometry.

References
DETERMINATION OF TOTAL AND BIOACCESSIBLE FRACTION OF Ba, Cu, Fe, Mn AND Zn IN STRAWBERRY

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Strawberry is produced and largely consumed in Brazil because of its nutritional value and flavor. However, the concentration of essential and toxic elements in the soil has been growing, stemmed of fertilizers, atmospheric pollution, rains and industrial wastes and the strawberry fruit has showed to accumulate a great amount of these elements, consequently it may cause risks to human consumption, depending on the magnitude of this consumption and on the elements absorption by the human body [1]. Therefore, the bioaccessibility studies are being developed in order to allow a better assessment of elements levels in several food samples. In these studies, the bioaccessible fraction refers to the amount of the compound or element that is released from the food matrix, which is soluble in the gastrointestinal tract and might be available for absorption by the intestinal epithelium. Thus, the objective of this work was to evaluate the total concentration and bioaccessible fraction of some elements in strawberry samples.

The quantification of total concentration by ICP OES was carried out after a microwave oxidative digestion. Approximately 5 g of in natura samples were mineralized with 5 mL of HNO3 and 3 mL H2O2. The extraction procedure simulating the gastrointestinal digestion was adapted from a model proposed by Minekus et al. [2]. Total elements released by gastrointestinal digestion were also determined by ICP OES through direct introduction of the supernatant obtained in the procedure. The results for the total concentration of Ba, Mn, Cu, Zn and Fe showed values of approximately 3.0; 3.7; 0.2; 1.3 and 7.4 mg kg⁻¹ respectively, and the bioaccessibilities were around 86; 73; 48; 29 and 20% of the total concentration. The high value for bioaccessible Mn might probably be due to the polyphenols content found in strawberries that may carry the element to the soluble fraction during the gastrointestinal digestion. The high values for Ba are harmful considering the toxicity of this element, causing risks to human health. The results also show that the half of Cu present in the fruit is bioaccessible while the values for Zn and Fe are much lower. These poor bioaccessibility for Zn and Fe were expected, since these elements tend to form insoluble compounds with phytates and fibers present in fruits while Cu may form Cu-phytate complexes more soluble in the gastrointestinal tract [3]. These results for Fe and Zn are critical, because both elements are essential for many physiological functions and should generally be ingested in higher quantities.

References

Acknowledgements: Casadinho Project/CNPq (Process nº 552197/2011-4), CAPES, Fapergs, Fapesp, INCTAA.
Selenium speciation is very important for environmental and human health. The toxicity of Se(IV) is more than Se(VI) [1]. Recently room temperature ionic liquids are interesting alternatives to organic solvents because of their unique physicochemical properties, which depend on the nature and size of their cationic and anionic constituents [2]. In this study, a new selenium speciation procedure has been optimized. Detection of analyte ions was performed by using graphite furnace atomic absorption spectrometry. Various analytical parameters such as pH, amount of ligand, volume of ionic liquid, extraction time, etc. were studied and optimized. Matrix effects of alkali, alkaline earth, some cations and anions were investigated. Low detection limit and high enhancement factor were obtained. Relative standard deviation (RSD) of the method was 5%. The accuracy of the method was confirmed with certified reference materials. Optimized method was applied to natural water samples for Se(IV) and Se(VI) speciation. Total selenium was determined in microwave digested food and environmental samples.

References

Acknowledgment
Dr. Mustafa Tuzen thanks to Turkish Academy of Sciences for financial support.
Environmental mobility and biological impact of potentially toxic elements (PTE) is determined by the chemical speciation of these elements in the system. According to recommendation of IUPAC Committees [1] speciation means the quantitative distribution of the given elements among its chemical species identifiable in the system. Therefore total risk assessment of contaminated areas should be based on total speciation of contaminant elements. The increased frequency of pollution events during the last decades of XXth century strongly stimulated the development speciation analytics, but simultaneously it has emerged that the total speciation is unreliably high analytical task in the practice. As a compromise the fractionation techniques were developed in which the solvents (reagents) modeling the pathways of environmental mobilization are applied sequentially for extraction of PTEs from solid environmental samples. In Europe mostly the simplified extraction scheme proposed in 1993 and modified in 2001 is widely used [2]. Up to now this is only the fractionation procedure to which a certified sediment sample (BCR 701) was issued. By the BCR procedure the chemical structures of sediment or soil samples are gradually decomposed and by this way the following fore fractions of PTEs can be distinguished: (1) Water-soluble and carbonate-bound fraction; (2) Associated with reducible iron- and Mn-oxides; (3) Organic complexed and sulphides; (4) Soluble in oxidative acids. Standardization of this procedure, however, up to now was hindered by the following methodological problems: (1) The solvents applied in the BCR system do not model the natural mobilization processes and do not keep the intact species forms. (2) Time demand of the batch leaching extraction steps is too long (4-5 days). (3) Only for sediments is available a CRM sample which is certified for fractionation of six elements (Cu, Cd, Cr, Ni, Pb, Zn), therefore the extension of validation for other environmental matrices (soils, solid wastes) and more PTEs is limited. In the lecture a survey will be presented on the results of our researches directed to solve the above problems: (1) Elaboration of continuous flow system for sequential extraction of water soluble and carbonate-bound PTE fractions; (2) Acceleration of BCR leaching steps by sonication; (3) Extension of BCR procedure to further environmental matrices (soils, red mud, composts, biofilms) and further PTEs by multielemental ICP-OES detections. The improved methodologies were applied for estimation of long-term change of environmental mobility of PTEs at two contaminated area (Upper-Tisza 2000/2014 and Gödöllő fishpond system 1995/2014).

References

Acknowledgement: This work was supported the Hungarian Scientific Research Fund (OTKA 108558).
ACCELERATION OF SEQUENTIAL EXTRACTION PROCEDURES OF POTENTIALLY TOXIC ELEMENT (PTE) CONTENT OF SOILS AND SEDIMENTS BY SONICATION

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For characterization PTE content in solid environmental samples (soils, sediments, wastes, etc.) now several methods are available, as the routinely used one-step extraction and quite complex sequential extraction methods. The great advantage of sequential extractions is that we can recognize new chemical information by sequential application of extraction reagents with gradually increasing chemical aggression at each step. However, in the generally applied batch leaching techniques require long time shaking to achieve the extraction equilibrium and therefore when a large number of samples should be processed the methodology is very time-consuming. To improve the time-effectivity of this methodology, a study was performed whether by ultrasound treatment could be influenced the extraction ability of solvents applied in extraction steps.

As a model task the widely used BCR sequential extraction[1] procedure was selected, which has been very efficiently used in the environmental analytics, because it provides relevant information on environmental mobility of all PTE-species present in the sample. The experiments were performed on the BCR-701 sediment sample, which is certified to BCR-procedure. The BCR protocol prescribes the application of the following solvents:

1. Step: 0.11 M CH₃COOH – 16 h shaking;
2. Step: 0.5 M NH₂OH×HCl – 16 h shaking;
3. Step: after H₂O₂-digestion, 1 M NH₄OAc – 16 h shaking;
+ 1 Step: HNO₃ / H₂O₂ microwave digestion.

In order to determine the satisfactory extraction time of each batch leaching steps three different treatment were applied: shaking (according to BCR-protocol), sonication and combination of both. In the “A” control-experiment the shaking agitation time was applied corresponding to the BCR-protocol, while in experiment “B” shaking time was set to one hour combined simultaneously with one hour of sonication, in experiment “C” only 1 hour ultrasonic treatment was used. We examined how the amount of releasable element was affected by the duration of the shaking and of ultrasonic treatment compared to the 16-hour shaking process. In case of 1 hour ultrasonic treatment only 72% of the PTE amount of regular BCR extraction came be dissolved and in the case of combination of 1 hour shaking and sonication it is reached the 83% of PTE amount dissolved by regular BCR extraction.

This research was supported by the Hungarian Science Research Fund (OTKA 108558).

Reference
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CLEANING PROCEDURES AND RELEVANCE OF HAIR ANALYSIS

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As a helpful environmental bioindicator, hair (fur) can demonstrate the organism load with various persistent bioaccumulative or doping substances and heavy metals. If stably built in the protein structure, these substances can be released after the irreversible destruction of the hair. Chemicals originating from the environment trapped on hair surface need to be removed by a washing process prior to analysis. Difficulties, unclearness and irreproducibility in results often come from a cleaning step prior to sample preparation. Although previous studies presented and recommended many washing procedures, only one unified IAEA procedure (using acetone and water) has existed. Especially washing steps bring potential risk of disruption of the hair internal structure and releasing of substances that are the subject of analytical interest. Therefore, the washing procedure used needs to be considered very carefully.

Properties of washing procedures used before hair analysis were studied. The plan of experimental work was built up using of statistical methods of design of experiment. The effect of single useable cleaning media (nitric acid, acetone, Triton X-100, EDTA) was tested in a model based on a full factorial experiment, four factors at two levels. The optimization of cleaning conditions (temperature, time, and agitation support) was assessed using a full factorial experiment, three factors at three levels. 15 elements were followed (ICP-OES) including these which set up the border between exogenous (sodium, potassium) and endogenous (sulphur, copper) indicators.

Significant differences between cleaning agents were found: each of them revealed different washing strength for specific elements. Surface impurities but also elements from the inner hair structure were removed (e.g. acetone released sulphur from the protein structure). Results brought more questions than answers:

– to compromise a washing step before multielemental analysis or to use the procedure tailored to a single element,
– comparability and relevance of data published in the literature,
– information capability of hair analysis with regard the washing procedure used, etc.
To further expand the area of optoelectronic applications, ZnO can be doped with different dopants. Therefore, researchers are making intensive research on the physical properties of the doped ZnO films [1-5]. In order to investigate the influence of dopant such as magnesium (Mg), boron (B), lithium (Li), cadmium (Cd), Fluorine (F), sodium (Na) content on structural and optical properties of ZnO films, all the ZnO films were prepared by facile solgel method using spin coating technique. Zinc acetate dihydrate, 2-methoxyethanol and mono-ethanolamine were used as a starting material, solvent and stabilizer, respectively. The dopant sources are used in salt formed. The influence of different dopant elements on the crystalline structure and orientation of the ZnO films have been investigated by X-ray diffraction (XRD) study. The structural parameters of the films were determined and compared. A double beam UV-vis spectrophotometer with an integrating sphere was used for the optical transmittance and diffuse reflectance measurements, respectively. At the visible region, the average optical transmittance values of all the films are greater than 80%. The values of absorption band edge were determined different optical methods such as Kubelka-Munk, Tauc methods. The optical constants (complex refractive index and dielectric constants) of the films were calculated using transmittance and diffuse reflectance spectra.

Figure 1. (a, b) SEM images and (c,d) The plot of optical transmittance (inset) and its first derivative of Mg and Na doped ZnO films, respectively.

Acknowledgement: This work was supported by Anadolu University Commission of Scientific Research Project under Grant No. 1305F082.

References
THE EFFECT OF FIREWORKS ON THE ELEMENTAL CONCENTRATION OF DUST DEPOSITED ON TREE LEAVES

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Explosive pyrotechnic devices are widely used for celebrating specific events. The quality and composition of these are strictly regulated by the law in Hungary. At the same time fireworks events are unusual sources of air pollutants since metal particles, different organic compounds and gases access the atmosphere during the explosions.

In the city of Debrecen the bank holiday of 20th of August is celebrated by fireworks show. The event is organized at the same time in two different locations. Our aim was to investigate the effect of the fireworks display on the quantity and the elemental concentration of dust particles collected from tree leaves.

The collection of control samples took place a few days before the event from the individuals of the selected species (Tilia tomentosa), while the trees were indicated and the coordinates were registered. Sample collection from the same 41 individuals was replicated after the fireworks event. Deposited dust particles were removed from the surface of the collected leaves mechanically and their mass was determined. Dust samples were acid digested prior to analysis. The elemental analysis of dust particles was carried out by ICP-AES (inductively coupled plasma atomic emission spectrometry) and MP-AES (microwave plasma atomic emission spectrometry) methods. Evaluation of the gained data were carried out by principal component analysis (PCA) for which the two sampling sites were further divided into 5-5 areas by the points of the compass. We studied the change in the amount of dust deposited on the surface of the leaves and in the determined Ca, Mg, K, Mn, Cu, Zn, Fe, Al, Ba, B, Li, As and Sr concentrations of the samples collected before and after the fireworks event.

According to the statistical analysis significant differences were observed in the amount of dust deposition after the fireworks event. A statistically higher level of Ca, Mg, and Sr was detected in samples collected after the display compared to those collected during the previous days, while the concentration of other studied elements were not statistically different from the background level.
Solid phase extraction technique has been widely used in the separation of trace/ultra trace amounts of inorganic and organic species, in order to enhance sensitivity and to separate analytical matrix. Nowadays, investigation of the usage of new materials as solid phase extractor is an important ratio to obtain environmental friendly, economic, fast, reliable determination of trace/ultra trace metals.

We report on the separation/removal of Cd, Cr, Cu, Pb and Co ions using peptide-coated gold nanoparticles and their determination by graphite furnace atomic absorption spectrometry. The ions were adsorbed via a conventional batch technique. The effects of peptide type, pH, amount of sorbent and capacity of the sorbent on the recovery were investigated. Under optimized experimental conditions, the analytes were recovered within the uncertainty limits of the certified value of a certificated reference sea water solution. In addition, the concentrations of analytes added to sea water were quantitatively recovered. The technique is fast, simple and environmentally friendly. The limits of detection (3σ, at n=10) were found 2.7 µg/mL, 0.8 µg/mL, 1.6 µg/mL, 1.1 µg/mL and 0.9 µg/mL for Cu, Cr, Cd, Pb and Co, respectively.
A COMPREHENSIVE STUDY OF THE NON-FERROUS METALS ARTIFACTS FROM THE ZAPOLOTSKI POSAD OF ANCIENT POLOTSK

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Nowadays, the study of medieval jewelry is one of the most urgent tasks for Belarusian archaeological science. Typological, stratigraphic, iconographic methods are the most widely spread as the traditional approaches to the study of the artifacts. However, the comprehensive study of archaeological materials with the help of techniques from the natural sciences is very crucial.

Several non-ferrous metal artifacts that have been discovered in Zapolotski Posad of ancient Polotsk in 2013 [1] were selected as the subject of the study. In the results of traditional approach the traces of the jewelry manufactory of the XII century have been found. To establish a specialization of the jewelry production and also the features of the using of the alloys the analytical study of the chemical composition of the artifacts have been carried out with the help of LIBS and ICP-MS techniques.

According to the obtained results the artifacts from the lead bronze (3 items), lead-tin bronze (2 items), multicomponent bronze (3 items), “pure” lead (4 items) and multicomponent brass (5 items) are presented in the collection. The particular attention should be focused on the billet metal as well as metal surfacing inside the ladle for casting. The traces of the multicomponent brass with low zinc content have been identified inside the ladle for casting and the lead bronze have been identified in the billet. Both alloys are characteristic for Polotsk jewelry production and frequently detected among Polotsk artifacts [2]. So, these results allow us to make conclusion about manufacture specialization on the certain kinds of alloys.

References
ANALYSIS OF THALLIUM IN SPRUCE NEEDLES USING SOLID SAMPLING-HIGH-RESOLUTION CONTINUUM SOURCE GF AAS

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Commercial use of thallium (alloying element, electronic industry, special refractive glass etc.) is limited due to its toxic properties. Owing to the industrial processing, Tl is emitted to the environment. Anthropogenic sources of Tl are mostly related to coal combustion, metal smelting, refining processes, and cement industry that is considered to be its largest emitter. Chemical analysis of Tl in plant bioindicators (grass, moss, litchen, occasionally coniferous needles) has been used in biomonitoring programmes for many years. Because of very low, ultratrace, natural concentrations of thallium in majority plant samples, highly sensitive analytical methods are required (ET-AAS, ICP-MS etc.) [1].

This work investigates the potential of high-resolution continuum source graphite furnace molecular absorption spectrometry with solid sampling for analysis of thallium in spruce needles. Sixteen samples (Czech Republic and Italy) of needles of spruce twigs were cut, dried in a laboratory oven homogenised with a cryogenic mill in liquid nitrogen (the final volume diameter of sample particles was about 15 µm). The treated spruce needles were analysed as solid samples by the HR-CS-AAS instrument ContrAA 700 (pyrolytic graphite tubes and solid sampling graphite platforms, the spectral line 276.786 nm) connected with the sampling unit SSA 600 (both Analytik Jena AG, Germany). It was dosed 10 µl of 1 g·l⁻¹ Pd(NO₃)₂ as a modifier and 1-2 mg of sample into the graphite platform. The temperature of pyrolysis/atomization was 1000/2000 °C. The certified reference material BCR-678 was analysed in order to validate the developed method: the obtained concentration of Tl 0.003 ±0.0002 μg·g⁻¹ was in the range of the certified value: 0.003 ± 0.0003 μg·g⁻¹, R = 98.9%. The limit of detection of the analytical method for Tl in needles sample was 0.001 μg·g⁻¹, RSD for the method was about 4%. The found concentrations of Tl in spruce needles ranged from 0.002 to 0.131 μg·g⁻¹, RSD (0.87-3.4 %). The proposed method seems to be suitable for the fast and simple control of these types of samples, overcoming the traditional problems associated with sample digestion (e.g., losses of volatile compounds).

References
INNOVATIVE NATURAL DEFATTING AGENTS: STUDY OF THE INTERACTION WITH LEATHER PROTEINS AND MONITORING OF THE ENVIRONMENTAL IMPACT

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Leather manufacturing combines several working phases that transform waste materials of the cattle industry such as animal skins (or hides) into valuable products such as the leather goods. Leather defatting is an important preparatory step prior to tanning. If fat is not taken away efficiently, the tanning agents cannot work properly within the molecular structure of the leather (i.e., the collagen and other fibrous type proteins) leading to poor quality material susceptible to thermal and mechanical degradation overtime. On the other hand, if the removed fat is too much, the leather becomes stiff and fragile, leading to tears and rips. Therefore, a good balance of defatting is required, to allow the stabilization of the skin into leather by the tanning agents, whilst keeping the softness and smoothness of the original animal skin.

Chlorinated paraffins and alkyl phenol derivatives were common defattting agents employed in the leather industry but in the last decades, they were replaced by ethoxylated long chain because of their environmental impact and hazards to human health. Nevertheless, the biodegradability of ethoxylated alcohols may be an issue, since branched ethoxylated alcohols tend to accumulate overtime and linear compounds may be degraded slowly. This context could become even more problematic, since degreasing agents contain also ethoxylated derivatives of vegetable oils and sugars, having the role of assisting the action of the ethoxylated alcohols. The result is a complex mixture of chemicals that are quite difficult to manage downstream, when effluents are discharged.

To simplifying the complexity of the commercial products and reduce the environmental impact of defatting effluents, new defatting agents based on the elaboration of the naturally occurring lactose, a waste substance of the dairy industry produced in hundreds of thousands of tonnes per year, were developed.

In this work we have used Attenuated Total Reflectance- Fourier Transform Infrared Spectroscopy (ATR-FTIR) and Thermogravimetric Analysis (TGA) for the study of natural defatting agents/leather protein interactions at molecular level.

The monitoring of the environmental impact of defatting effluents from the use of new formulations was carried out through the metal analysis performed with Inductively Coupled Plasma Mass Spectroscopy (ICP-MS), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and Direct Mercury Analyzer (DMA).

To comparison, also some commercial products were analyzed. We have demonstrated the effective capability of some of the developed natural compounds to replace the commercial products and reduce the environmental impact of defatting effluents.

Acknowledgments

Life + EU Project ENV/IT/000470 “ECODEFATTING”
SOLID SAMPLING DETERMINATION OF MG IN LiNbO3 CRYSTALS
BY HIGH RESOLUTION CONTINUUM SOURCE ATOMIC
ABSORPTION SPECTROMETRIC METHOD

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The application of the widely used nonlinear optical LiNbO3 crystal is often limited by the
photorefractive effect, facilitating laser induced damage of these materials. Increased optical
damage resistance can be obtained by doping the crystal with MgO above a threshold
concentration [1]. Several physical properties, like IR OH band- [2] and UV-edge position
[3], and also the laser damage threshold, show an abrupt change in crystals doped with MgO
above the threshold. For this reason and for the optimization of crystal growth, the
determination of the Mg concentration in LiNbO3 crystals is essential.

Comparing the methods for the determination of the Mg content in LiNbO3, the direct
analysis of solid samples has several advantages over procedures involving acidic digestion
or other dissolution methods [4], because it is less time-consuming, since only a minimum of
sample preparation is required, more sensitive, since the Mg content is not diluted during
sample preparation and the risk of Mg loss and contamination of the sample is reduced to a
minimum.

In this study, the direct solid sampling determination of Mg dopant in LiNbO3 crystals
was developed using high-resolution continuum source graphite furnace atomic absorption
spectrometry (HR-CS-GFAAS). The vaporization/atomization processes were investigated
in a transversally heated graphite atomizer by evaporating solid samples of LiNbO3 crystals
having different Mg content. The best results were obtained by using the Mg I 215.4353 nm
secondary analytical line. The maximum (optimal) pyrolysis temperature of 1500 °C has
been found, and the optimum (compromise) atomization temperature was 2400 °C. The
correlation coefficients (R values) of the calibration curves were found to be 0.9999. The
upper limit of the linear calibration range was 4.5 mol% Mg content. The Mg content in the
solid samples was found to be in the range of 1.06-2.02 mol%.

References
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Increased concentration of toxic elements, such as cadmium (Cd) in water, soil and air is mostly caused by anthropogenic activity. Analyzing the content of Cd in tissues of some species of plants and animals we can obtain the information about the quality of the ecosystem in which animals live. Game animals, constantly exposed to environmental factors, may be used as biomonitors of environmental metal levels. The objective of presented research was to assess environmental pollution by Cd using wild boar (*Sus scrofa*) as biomonitor. The research was carried out in four industrial regions in Poland: Turoszow Coal Basin, Belchatow Brown Coal Basin, Legnica-Glogow Copper District and the area of Zinc Smelter Miasteczko Slaskie located in Upper Silesia. The Masurian Lake District was chosen as the reference site. A total of 320 animals were shot according to regular hunting plans in the period from October 2011 to February 2013. The samples of muscle, liver, kidney and hair of wild boar were collected after shot and stored at -20°C until analysis.

Concentration of Cd was analyzed by graphite furnace atomic absorption spectrometry (GF-AAS) after mineralization of samples in muffle furnace at 450°C according to previously described method. All results are expressed in wet weight. Our result show that the highest concentrations of Cd in tissues and hair of wild board were found in the area of Upper Silesia which appears to be the most contaminated due to the activity of lead-zinc smelter. The median concentration of Cd in muscle tissue ranged from 0.003 in the reference area to 0.028 mg/kg in Upper Silesia. Concentration of Cd in liver ranged from 0.151 to 3.694 mg/kg; in kidney 2.115 - 37.61 mg/kg; in hair: 0.048 - 0.633 mg/kg. Significant positive correlations were found between concentration of Cd in hair and muscle (r=0.259, p=1.51×10^{-5}), hair and liver (r=0.240, p=5.96×10^{-5}) and hair and kidney (r=0.232, p=1.14×10^{-4}). The association found between Cd content in hair and tissues confirmed that this matrix may be used as non-invasive bioindicator of Cd level. The maximum levels of Cd in meat, liver and kidney of slaughtered animals specified in Commission Regulation (EC) 1881/2006 was exceeded in 5, 34 and 94% of muscle, liver kidney samples respectively. High levels of Cd in the offal of wild boar may pose a threat to the health of the consumers of venison, particularly hunters and their families.

**Acknowledgments**

The research was supported by the National Centre for Research and Development in Poland, project No. 12-0127-10 and co-financed by KNOW (Leading National Research Centre) Scientific Consortium “Healthy Animal - Safe Food”, decision of Ministry of Science and Higher Education No. 05-1/KNOW2/2015.
AN APPLICATION OF THE PROGRAMMABLE THERMOSTATED SPRAY CHAMBER FOR DIRECT CHEMICAL VAPOR GENERATION IN ICP-OES AND MIP-OES

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Conventional method of solution nebulization with the use of a pneumatic nebulizer and a cyclonic spray chamber allows for only several percent efficiency of aerosol transport to the plasma that affects the sensitivity of analytical method used. A new approach in this matter is the use of a programmable temperature spray chamber (PTSC) system. The device enables precise temperature control of the spray chamber in the range from -10 to +60°C via Peltier system. It has been shown that chamber temperature significantly affects total solvent transport efficiency to the plasma. For pneumatic nebulization and the PTSC temperature of 0°C transport efficiency was approximately four times smaller than at 50°C[1,2].

By taking advantage from temperature optimization the presented sample introduction system becomes more versatile and allows for stable and controlled sample introduction that improves the measurement precision and signal-to-noise ratio. The PN-PTSC system has found a new and interesting application by coupling with direct vapor generation (CVG) techniques. Importantly, both PN-PTSC and CVG-PN-PTSC techniques can be realized practically with the use of the same sample introduction system[3].

Presented results include those obtained by chemical vapor generation of iodine, hydride generation of selenium, arsenic, antimony and cold vapor generation of mercury combined with ICP-OES (Inductively Coupled Plasma Optical Emission Spectrometry) and MIP-OES (Microwave Induced Plasma) techniques [4]. Also, two different types of nebulizers, namely pneumatic and ultrasonic, have been investigated in order to perform complex study.

Generally, increase of PTSC temperature causes more effective transport of solvent to the plasma so the effect of plasma overloading occurs in more vulnerable sources such as low-power MIP or low power ICP. For these sources lower temperature is recommended, while for robust ICP (1200W), temperature settings near 50°C seem to be the best choice, where high sample loadings reach the plasma. Interestingly, the analytes examined in this study exhibited different responses to the PTSC temperature changes that might be explained by distinct features of vapor generation reactions leading to the formation of hydrides or elemental and molecular vapor. With PTSC, the figures of merit by ICP-OES and MIP-OES are improved by a factor of 2-100 for all analytes studied comparing with those by ICP-OES and MIP-OES with conventional solution nebulization. The LODs obtained for ICP and for As, Se, Sb, Hg and I were 5, 5.4, 2.7, 0.085 and 9 µg·L⁻¹, while for MIP they were 20, 14, 19, 2.5 and 8 µg·L⁻¹, respectively.

References
EFFECTS OF ANTHROPOGENIC ACTIVITIES ON SEDIMENT CHEMISTRY IN LAKE VELENCE (HUNGARY)

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Many anthropogenic activities have negative effect on aquatic ecosystem. We found that the heterogeneity of the Lake Velence (Hungary) disappeared because of anthropogenic activities. There are three characteristic parts of the lake based on water chemistry parameters: the so-called black, grey and green water. The nature reserve area is the black water; the middle of the lake is the grey water, and the Eastern part of the lake is the green water. The aim of our work was to study the heterogeneity of Lake and the assessment of the anthropogenic activities on the elemental concentration based on sediment using correlation between organic matter content and elemental concentration. Sediment cores were collected from the nature reserve area (Német-tisztás), middle of the lake (Lángi-tisztás), and Eastern part of the lake (Öreg-tisztás). The sediment cores were one meter long in all sampling areas; the sediment cores were cut to 2 cm subsamples. In each subsamples organic matter content was measured and the following elements were analysed with MP-AES: Al, Ca, Fe, K, Mg, Mn, Ba, Cr, Cu, Na, Pb, Sr and Zn. The three sampling areas were separated from each other based on elemental concentrations and organic matter content of sediment cores using canonical discriminant analysis (CDA). Little overlap was found between Német-tisztás and Öreg-tisztás, and between Lángi-tisztás and Öreg-tisztás. For all elements and also for the organic matter content significant differences were found among the different parts of Lake. Significant negative correlation was found between organic matter content and Al, Ca, Fe, Mg, Mn and Cr concentration which indicated that these elements were associated with the mineral parts of the surface. Thus, the source of these elements may not anthropogenic. The organic matter content correlated positively with the Ba, Cu, Na, Pb and Sr concentration, which indicated that the source of these elements may be anthropogenic activity. Our results demonstrated that the Lake Velence is composed of three parts based on the elemental concentration of sediment similar to the water chemistry. Our result also demonstrated that anthropogenic activities have significant effects on the elemental concentration of sediment.
CHARACTERIZATION OF A SPARK DISCHARGE PLASMA USED FOR COPPER NANOPARTICLE GENERATION

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Spark discharges have been widely used as plasma sources for atomic emission spectrometry [1]. Schwyn et al. was the first to prove that sparking is also an effective and versatile way of producing nanoparticles (NPs) [2]. In the conventional setup of a so called spark discharge generator (SDG) the discharge is fed by a bipolar, capacitor charging circuit producing repetitive sparks between the electrodes [3]. Thermal evaporation and sputtering erode the electrode material which leads to NP formation in the surrounding, flowing gas. In the present study the atomic emission of the spark plasma is used to characterize the discharge when Cu NPs are generated in Ar, in order to support the understanding of NP formation mechanisms.

The light of the emitting plasma is imaged onto the tip of an optical fiber connected to an Echelle spectrograph equipped with a high sensitivity ICCD camera. The setup allows for the collection of the 300-800 nm spectral and 70 ns – 50 μs temporal ranges with a spectral, temporal, and spatial resolution of ~0.1 nm, 500 ns, and approx. 50 μm, respectively. The temporally and spatially resolved atomic emission spectra is used to define the spatial dimensions of the emitting volume, as well as to describe the variation of plasma parameters, such as the temperature and the concentration of various plasma components.

During the breakdown phase of the discharge, a conducting plasma channel – predominantly consisting of electrons and argon ions – bridges the electrodes. This spatially concise channel is maintained for about 5 μs by the electric current flowing through the gap. The equilibrium temperature of Ar⁺ ions in the channel is in the order of 20000 K, while the electron concentration decreases from 7 to 2×10¹⁷ cm⁻³ as time passes. When the current is ceased, the cylindrical shape of the plasma is no longer kept and the temperature drops to ~9500 K with a concomitant decrease in the electron concentration to ~1×10¹⁶ cm⁻³. The concentration of Cu ions and atoms exists in the gap is in the order of ~1×10¹⁴ cm⁻³.

Acknowledgement
This project has received funding from the European Union’s Seventh Framework Program (FP7/2007-2013) under grant agreement no. 280765 (BUONAPART-E) and from the TÁMOP programme of Hungary (No. 4.2.2.A-11/1/KONV-2012-0047).

References
DETERMINATION OF ALKALINE ADDITIVES IN YTTRIUM OXYORTHOSILICATE BY SOLID SAMPLING HR-CS-GFAAS

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Yttrium oxyorthosilicate crystals doped with cerium (Y$_2$SiO$_5$:Ce) are blue phosphor scintillator materials, which has been applied in medical imaging devices [1]. These refractory materials are fabricated in low amounts (a few hundred milligrams) by means of flux-assisted, high-temperature fusion in the authors’ lab. In these syntheses, the method of Li$^+$/Na$^+$ co-doping in the flux is usually applied to enhance optical efficiency of the crystals, which is a well-accepted strategy in the research of oxide-based materials [2]. Li and Na additives, applied as fluorides, can build into the lattice of the Y$_2$SiO$_5$ host crystals, thus they can modify the luminescence intensity [3]. Consequently, the accurate determination of these elements is of great importance for the optimization of the synthesis procedure and to provide information for supporting the results of the crystal-physical/chemical investigations.

This study reports on the elaboration of solid sampling high resolution continuum source graphite furnace atomic absorption spectrometry (SS-HR-CS-GFAAS) methods for the fast and sensitive quantitation of Li and Na additives in microsamples of yttrium oxyorthosilicate scintillator materials. In these experiments, we applied an Analytik Jena Model ContrAA-700 tandem HR-CS-AAS spectrometer (Analytik Jena AG, Jena, Germany) equipped with a transversally heated graphite atomizer, a furnace video-camera, and Model SSA-600L and MPE-60 autosamplers for solid and liquid samples, respectively. The methods were optimized for solid (powder) sampling by studying a set of GFAAS conditions, such as sample mass, sensitivities of alternative analytical lines, and graphite furnace heating programs. For analytical purposes, the powdered Y$_2$SiO$_5$ samples in the mass range of around 0.1-0.4 mg were dispensed onto graphite sample insertion boats, weighed on the built-in microbalance of the SSA-600L and then analyzed. The pyrolysis and atomization temperatures were firstly optimized by recording the pyrolysis and atomization curves by the use of Li and Na single-element standard solutions at Li I 610.353 nm and Na I 285.3013 nm. Then the pyrolysis and atomization curves were also recorded by the use of powdered solid samples, in order to get an insight into the vaporization characteristics of analytes from powdered Y$_2$SiO$_5$. For quantitation of Li and Na in the solid samples, the method of standard addition calibration was applied. The correlation coefficients (R) of the linear fittings to the calibration points were not worse than 0.983. The detection limit for solid samples was 20 µg/g Li and 80 µg/g Na. The alkaline content of the solid samples were found to be in the range of 0.89 and 8.4 mg/g. The accuracy of the results obtained with the present solid sampling methods was verified by means of analyzing certified reference samples, using methods of standard (solution) addition calibration.

References
The study of evaporation process of solid samples means the first step within the optimization and validation of optical emission spectrometry method (OES) which use inductively coupled plasma (ICP) as an excitation source and graphite furnace for electrothermal evaporation (ETV) as an evaporation device. According to applied spectrochemical additives (AgCl, Li$_2$CO$_3$), values of relative intensities of chosen potentially toxic elements (Cd, Cr, Ni, Pb) as well as values of half-time of evaporation ($t_{50\%}$) and values of total evaporation time ($t_{100\%}$) were evaluated using model samples with composition similar to environmental samples (sediments). Study of evaporation process was completed by evaluation of relative standard deviation values (RSD). Application of AgCl was found out as the most suitable to achieve high-efficiency of evaporation of analytes directly from solid samples (SS). Positive influence of AgCl was observed in case of signal intensity, signal stability (RSD) and kinetics of evaporation, while the Li$_2$CO$_3$ additive seems to be the least suitable according to incomplete evaporation resulted in low signal intensity, unsuitable kinetics of evaporation and high RSD values. According to evaluation, spectral lines of potentially toxic elements suitable for trace analysis by validated SS-ETV-ICP-OES method were specified.

Keywords: solid sampling, ETV-ICP-OES, evaporation, heavy metals

Acknowledgements
Authors are grateful for the support of experimental works by project VEGA 1/0126/14.
CALIBRATION AND STATISTICAL DATA EVALUATION IN DIRECT SOLID SAMPLING METHODS

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One of the main uncertainty sources and in the same time – reason for biased results is the sample preparation procedure. In most of the cases it implies dissolution and wet mineralization of the sample. One of the contemporary solutions of the sample preparation problems is the application of analytical methods involving direct solid sampling.

Direct sampling/analysis of solid state materials creates specific difficulties:
– It is impossible to provide and measure correct solid phase procedural blank. Usually it is replaced by instrumental blank or water.
– It is impossible to measure correct replicates, since the masses measured are always different.
– Calibration is performed using liquid standard solutions with different behavior in the analytical system. Statement for constant sensitivity for liquid and solid samples cannot be accepted as true in all cases.

Considering these suggestions method validation and establishment of metrological traceability of the results becomes challenging tasks.

The present work describes a new calibration technique based on the use of solid certified reference materials similar in nature to the analyzed sample. Analyte content and uncertainty evaluation, repeatability, limits of detection and quantifications (LOD, LOQ), and other validation parameters can be revealed using statistics related to the linear regression. Metrological traceability is a logical consequence of the calibration procedure. Advantages of solid phase CRM calibration are confirmed by comparison with conventional (default) techniques. Method validation is demonstrated as well.

The described method is demonstrated in case of SS-HR-CS-AAS determination of ecologically important trace elements in various environmental samples and CRMs and Hg direct determination in solid samples using Advanced Mercury Analyzer (AMA).

Besides the metrological advantages, the proposed calibration method allows use of fast temperature programs in case of AAS and AMA, shortened additionally by excluding (or reducing significantly) the drying step.

The presented method is potentially applicable also to Laser ablation (LA), Electro thermal vaporization (ETV) systems and other solid sampling methods.
SPECTROSCOPIC DETERMINATION OF METALLIC SPECIES IN ELECTROLYSIS MEDIA FOR INVESTIGATION OF UNWANTED ELECTRODE FOULING PROCESSES

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The electrochemical reduction of carbon dioxide is very much in the focus of interest today. Intensive research is carried out in leading laboratories trying to work out methods for making useful materials from this the unwanted greenhouse gas using solar or wind power generated excess electric energy. Since carbon dioxide is a main component of Martian atmosphere the planned expeditions to that planet would be easier if solar power generated fuel could be produced there.

Different working electrodes are used in the experiments. Among them ones made of copper, nickel or metal alloys are very popular. In our laboratory electrochemical reduction experiments are carried out in homemade cells supplied with high surface area metal electrodes. In these studies background electrolytes containing carbon dioxide absorbing components like monoethanolamine (MEA) or different ionic liquids are used.

It was noticed, that during electrolysis, the activity of the electrodes undergoes some changes. It was expected that some unwanted interactions between the electrode surface and the electrolyte responsible for this.

Metal containing species were noticed in the used electrolyte. Therefore parallel to the electrochemical measurements the metal components in the electrolyte were checked with atomic absorption methods for getting better insight to the nature of the electrode passivation.

In the presentation the results obtained will be discussed, and explanation of the surface reaction causing the electroactivity changes will be attempted.

Acknowledgements
The work is financially supported by the Hungarian National Research development and Innovation (NKFI), under grant OTKA: K 112699 „C0₂ content selection of biogases and industrial waste gases” project.
ANTIMONY IN BREAKFAST TEA - CHARACTERIZATION AND QUANTIFICATION OF HEAVY METALS IN FOOD PACKAGING

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In recent times, design, shape and sensation of tea bags on the shelves of retail stores has changed. It seems that some of them may be made of plastics.

In the food industry, the polymer PET (polyethylene terephthalate) is used widely for packaging materials and antimony (Sb) is used as a catalyst in the polymerization, the primary step in plastic production. From harmless to harmful, the effects of antimony and its compounds on human and environmental health differ widely. Can Sb and substances contaminate food products?

Non-destructive testing using FTIR (Shimadzu IRaffinity-1S equipped with a Specac Quest single reflection ATR) and ED-XRF (Shimadzu EDX-8000) gives clues about the material a tea bag is made of and the amount of Sb present in the tea bag. In addition, the highly sensitive ICP-OES technique (Shimadzu’s ICPE-9820 equipped with hydride ICP, ESI Elemental Scientific) has been applied for elemental analysis of the brewed tea and tea bags.

It was found that paper may be disrupted and lose its functionality after long immersion in hot water. The newer generation of tea bags is therefore made of plastics. Of course, tea bags are also still made of cellulose, but is it only cellulose? The industry develops a lot of hybrids.

It has been analyzed which further materials are in use and it has been shown that combining the results of different analytical spectrometric techniques gives more information. Diverse tea bags from different suppliers of tea have been analyzed and analytical data will be presented.
SPECIATION OF PLATINUM USING VARIOUS POSSIBILITIES OF 
ANALYTICAL SIGNAL ENHANCEMENT. 
COMPARISON OF AAS AND UV-VIS DETERMINATION 
OF PLATINUM

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Various possibilities of analytical signal enhancement were used for Pt determination as ion associate (IA) with SCN$^-$ and 1,3,3-trimethyl-2-[3-(1,3,3-trimethyl-1,3-dihydroindol-2-yliden)-propyl-1,3-dienyl]-3H-indolium chloride more known as Astraphloxine FF (APFF). The conversion of platinum IA allows the extraction of Pt from samples containing many elements such as Cu, Cd, Ni, Co, Cr, Pb, In, Ag, Pd, Ir, Rh, and Ru. In this case, platinum (II) is extracted in the form of IA under standard conditions, whereas platinum (IV) is extracted only after the initiation of IA formation by force of various sources of energy (thermal treatment, ultrasonic and microwave energy) in the test sample. In comparison with thermal treatment the use of ultrasonic power reduces the needed time from 30 min up to 5 min and microwave energy up to 45 s.

Optimized conditions of IA formation enabled the suggestion of speciation analysis of Pt(II) and Pt(IV). Species can be determined simultaneously in the concentration ratios from 1:5 to 5:1. IA are extractable by toluene or amylacetate up to volume ratio $V_{aq}: V_{org} = 50 : 1$. This fact decreases the LOD from 90 µg L$^{-1}$ to 5 µg L$^{-1}$ and from 7.1 µg L$^{-1}$ to 0.3 µg L$^{-1}$ (as Pt) of UV-Vis and AAS determination respectively. Proposed methods were used for Pt determination in artificial and real samples with reliable results.

Acknowledgements
This work was supported by the Scientific Grant Agency VEGA of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences VEGA Grant No. 1/0253/16, 1/0126/14.
STRAIGHTFORWARD DETERMINATION OF U, Th, AND Hf AT TRACE LEVELS USING ULTRASONIC NEBULIZATION AND AXIAL VIEW ICP OES

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Inductively coupled plasma optical emission spectrometry (ICP OES) was applied for direct determination of U, Th and Hf in environmental and geological samples (phosphate rock, soil, sediment, bush branches and leaves, and natural water). Several spectral lines and sample decomposition procedures were investigated with respect to spectral and non-spectral interferences. For U and Hf determination, the geological samples treatment required hydrofluoridric acid, whereas Th could be accurately determined in the samples decomposed by aqua regia solely. Ultrasonic nebulization (USN) and pneumatic nebulization with aerosol desolvation (PN-DES), with and without a microporous membrane, were evaluated for introducing the sample solution into the ICP. Better results were obtained by using USN; the limits of detection of U (U II 409.014 nm), Th (Th II 401.913 nm) and Hf (Hf II 264.141 nm) were 0.03, 0.01, and 0.01 µg g⁻¹, respectively, by using axial view ICP OES [1]. Uranium, Th and Hf were precisely and accurately determined without matrix separation/analyte pre concentration; the relative standard deviation (RSD) was typically < 7% and the recovery of the analytes in the certified reference materials (phosphate rock, soil, sediment, vegetal, and natural water) ranged from 83 to 112%. These results were linked to careful selection of spectral lines, which depended on the sample matrix and reagents used for sample decomposition.

References
The biological, microbiological and chemical analysis of human blood samples supports the field of medical diagnosis and research. The determination of essential and toxic elements in proteins enables the study of transport processes which carries useful diagnostical information.

Contrast agents are applied to improve the visibility of internal body structures since they interact more or less with the investigated tissue. In magnetic resonance imaging (MRI) paramagnetic gadolinium(III) complexes are commonly used contrast media that enhances the quality of MRI scans taken from the different organs and tissues.

In recent study Omniscan ([Gd(DTPA-BMA)] containing human serum samples were fractionated by DEAE Trisacryl M anion-exchange column and four proteins were identified by UV spectrophotometry: IgG, transferrin, albumin and ceruloplasmin. The gained protein fractions were digested with the mixture of concentrated nitric acid and hydrogen-peroxide. The Gd$^{3+}$ concentration of the protein containing samples were determined by inductively coupled plasma atomic emission spectrometry (ICP-OES, 5100 Agilent Technologies) method. The highest Gd(III) concentration was found in the fractions containing albumin and ceruloplasmin.

We would like to highly acknowledge Agilent Technologies (Novo-Lab Ltd.) for providing the ICP-OES 5100 instrument for the elemental analysis.
In this study, lead concentrations in various plastic toys were determined directly by solid sampling high resolution continuum source graphite furnace atomic absorption spectrometry. The toys were cut into small pieces and introduced into the graphite furnace between 0.05 and 0.7 mg without any further treatment. Lead was determined at 217.005 nm using a Pd+Mg modifier. Samples were pyrolyzed at 1000°C and atomized at 2200°C with or without gas flow at atomization stage depending on the concentration of the analyte. The lead concentration in a certified reference plastic material (ERM-EC680K) was determined in the uncertainty limits of the certified value. The limits of detection in gas-stop and gas-flow modes for 0.7 mg of sample were 0.037 and 0.93 mg kg⁻¹, respectively. The concentrations of lead in different colours plastic toys were found in the range of 0.060-9.12 mg kg⁻¹.
DETERMINATION OF Na, K, Mg, Ca AND Si IN BIOMASS SAMPLES AND THEIR PYROLYSIS PRODUCTS USING HR-CS AAS

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Biomass is an alternative source of energy, for example as bio-fuel that can be obtained from biological materials. In this work, samples of peach pit, palm oil (dende oil) and sugarcane straw were investigated. The raw biomass materials, the bio-oil, the aqueous phase and the biomass ashes, obtained in the pyrolysis process, were analyzed by high-resolution continuum source atomic absorption spectrometry (HR-CS AAS). The elements Na, K, Mg, Ca and Si were determined in the raw products and all intermediate and final products of the process, and a preliminary mass balance was established to estimate the fraction of the elements lost in the pyrolysis stage. The bio-oil samples were analyzed as micro emulsions. The adopted proportion of the components in the micro emulsion was: 67% (v/v) propan-1-ol, 22% (v/v) bio-oil and 11% (v/v) water / HNO₃. The raw biomass materials, the aqueous phase and the biomass ashes were analyzed directly. The objective of the work was to characterize the raw materials and their products. The use of HR-CS AAS presented the feasibility of sequential multi-element determination. The aim of this study was the development of an analytical method for the sequential determination of Mg, Ca, Na, K and Si in biomass samples by high-resolution continuum source flame atomic absorption spectrometry (HR-CS F AAS) and/or graphite furnace atomic absorption spectrometry (HR-CS GF AAS). Aqueous standard solutions and micro emulsions were used for calibration and the limits of detection (LOD) and quantification (LOQ) were established. Different approaches were applied to evaluate the accuracy of the proposed method, such as digestion procedures, recovery tests and analysis of certified reference materials.

Acknowledgments: CAPES and CNPq.
A NOVEL EXTRACTION-BASED PROCEDURE FOR THE DETERMINATION OF CADMIUM IN MARINE MACROALGAE BY HR-CS GF AAS

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Currently there are quite some discussions about the environmental changes, which are related, either directly or indirectly, to human activities. Many deliberations about the environmental impact of these activities have received media attention due to the loss of human lives and economic resources, but the impact on biodiversity of coastal areas, particularly marine macroalgae, has not received many meaningful dialogues [1]. Macroalgae can be found close to the ocean–continent interface, which is strongly influenced by human activities, such as industry, marine transportation, fishing and tourism [2]. An important parameter to analyze and monitor the impact of these activities is the metallic contaminants absorbed in macroalgae. The aim of this study was to optimize a new extraction procedure using only nitric acid, hydrogen peroxide and temperature for the determination of cadmium in marine macroalgae by HR-CS GF AAS. The extraction procedure has been optimized using a multivariate method of central composite design for three variables. Five levels of the variables, being the concentrations of HNO₃ and H₂O₂ and the extraction time at a temperature of 80 °C were studied, totaling seventy experiments. The optimized conditions were 15 min, 15% HNO₃ and 15% H₂O₂, totaling 2 mL completed with deionized water. Figure 1 shows the parameters optimization. The proposed method was applied to seventy marine macroalgae samples from the Fernando de Noronha Island, Brazil. The limit of detection and quantification were 0.1 and 0.3 µg g⁻¹, respectively. In order to assure the accuracy obtained for the analyzed samples, three randomly-selected samples were also analyzed by ICP-MS. Based on a Student t-test at a confidence level of 95%, no statistic difference was found between the results obtained from extraction by HR-CS GF AAS and those from ICP-MS analysis.

Figure 1. Response surfaces obtained from the central composite design for Cd signal. Variables are: extraction time at 80 °C, H₂O₂ and HNO₃ concentrations.

References
Taking account that both compositionally and structurally the samples are highly heterogeneous, archaeological iron slags can be categorized according to their technological origins (from bloomery furnace, blast furnace, puddling hearth, finery and/or smithy) and raw material provenance on the basis of their chemical and mineralogical composition and structural characteristics.

Two sets of iron slag probes unearthed at the Brâncovenești/Marosvécs and respectively Călugăreni/Mikháza sites, completed with a slag sample from the Vâtava/Felsőrépa site were studied by spectroscopic methods in order to determine their chemical composition and to establish the extent of their inhomogeneity.

Surface elemental measurements for characterization of samples inhomogeneity was performed with an INNOV-X Alpha-6500 handheld XRF spectrometer (spot size 2 mm², 35 kV, 15 μA, 3 mm filter, Be window, PIN Si detector).

The experimental data obtained confirm that when discussing on the chemical composition, consideration of the heterogeneity of the samples is mandatory.

Chemical analyses of the bulk composition were carried out using the previously presented handheld instrument and method (d=1 cm sample holder, 1 g of sample with the external weathered layer removed pulverized in agate mill), and, considering the necessity to obtain data for the lighter elements also, by ICP-OES (OPTIMA 5300 DV, Perkin Elmer).

In concordance with the expectations and supported by FTIR spectroscopic data, the results indicate that the main mineral phase of the samples is most probably fayalite.

FTIR spectra were obtained on KBr pellets in the spectral domain 2000 - 400 cm⁻¹ using a JASCO 6100 FTIR spectrometer of 4 cm⁻¹ resolution.

In order to have a look on the redox conditions in which the slags were formed, we tried to determine the Fe(II)/Fe(III) rate of the probes. In this purpose EPR experiments were performed at room temperature in the X-band (9.46 GHz) on a Bruker ELEXSYS E500 spectrometer.

The EPR spectra evidenced properly the presence of Fe³⁺ ions in the samples, however proper conclusions require the completion of the data by means of further investigations (thin section microscopy, XRD and others).

**Keywords:** iron slag, XRF spectrometry, ICP-OES, EPR spectroscopy, FTIR spectroscopy
EVALUATION OF HEAVY METAL TRACES (Pb, Cd AND Hg) OF SOME FISH SPECIES BY GF-AAS AND CV-AAS

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Fish is an important human food because it provides high quality proteins and is rich in polyunsaturated fatty acids. However, due to environmental pollution, toxic elements can accumulate in fish to such a high level to pose health risks to humans.

This study contributes to the evaluation of heavy metal concentrations {Cadmium (Cd); Lead (Pb) and Mercury (Hg)} present in 43 samples of 5 different marine species. Sardines (Sardina pilchardus), mackerels (Scomber scombrus and Trachurus trachurus), squids (Sepia officinalis) and octopus (Octopus vulgaris) were fished and disembarked at different ports of southern Morocco from the beginning of March until the end of May in 2014.

Concentrations of cadmium and lead were determined by a graphite furnace atomic absorption spectrometry (GF-AAS) and mercury was measured by automatic mercury analyzer by cold vapour generation (CV-AAS) after digestion of the consumable parts of the different marine species. The results showed that Cd, Pb and Hg were present in the samples with an average concentration of 29 ppb, 6 ppb and 30 ppb by weight/wet weight, respectively. The determined levels didn’t exceed the limits defined by international organizations like U.S. Food and Drug Administration (FDA), Codex Alimentarius or European Commission (EC). Based on our results the maximum allowable fish consumption rate was calculated (3 kg/week). This data, while based on a limited sample size and therefore further investigations are needed, nevertheless provide the basis for developing consumption guidelines in Morocco.
DETERMINATION OF Cd, Cr AND Cu IN VEGETABLES OF THE
SOLANACEAE FAMILY USING HIGH-RESOLUTION CONTINUUM
SOURCE GRAPHITE FURNACE ATOMIC ABSORPTION
SPECTROMETRY

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To recognize botanical families is useful, because they share both similar cultural
requirements and the same or similar pests. The solanaceae family comprises a large number
of frequently consumed vegetables, due to the large amount of nutrients and their delicious
taste. The goal of this work is the determination of Cd, Cr and Cu in samples of red, yellow
and green bell pepper, potato, tomato, eggplant, pepper and physalis using high-resolution
continuum source solid-sampling graphite furnace atomic absorption spectrometry (HR-CS
SS-GF AAS). The vegetables were lyophilized, grounded in a micro-mill and sieved. For Cd
determination, the atomic absorption was measured using CP±1 at the main line at 228.802
nm; a pyrolysis temperature of 1000 °C and an atomization temperature of 1500 °C, using
Pd-Mg as the chemical modifier. The characteristic mass (m0) and limit of detection (LOD)
were 0.42 pg and 0.78 ng g⁻¹, respectively. For Cr determination, the atomic absorption was
measured using CP±1 at the main line at 357,868 nm; a pyrolysis temperature of 1700 °C and
an atomization temperature of 2600 °C. The m0 and LOD were 2.7 pg and 2.5 ng g⁻¹,
respectively. For Cu determination, the atomic absorption was measured using only the
center pixel (CP) at 327.396 nm (45 % sensitivity) and a minimum gas flow rate during the
atomization stage, due to the high concentration of Cu; a pyrolysis temperature of 1100 °C
and an atomization temperature of 2400 °C. The m0 and LOD were 19 pg and 0.15 µg g⁻¹,
respectively. The accuracy of the proposed methods was verified using certified reference
materials (CRM). The values obtained for the CRMs were in agreement with the certificate.
The concentration was found between <LOD and 301 µg kg⁻¹ for Cd; 0.095 and 1.0 µg g⁻¹ for
Cr and between 4.5 and 18.4 µg g⁻¹ for Cu. Some vegetables are above the maximum limit
allowed by specific legislation.

Acknowledgments
CAPES and CNPq.
METHOD DEVELOPMENT FOR THE DETERMINATION OF Cu AND Mn IN INFANT FORMULAS BY HR-CS GF AAS USING DIRECT SOLID SAMPLE ANALYSIS

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Infant formulas are available in liquid or powder form and are produced with the aim to feed babies as an alternative for partial or total replacement of breast milk. Such products have a high nutritional content, such as vitamins and minerals, to supply baby’s needs. Metals, such as Cu and Mn, are considered essential micronutrients; however, their excessive intake can be toxic, becoming of great importance a fast and accurate analytical tool for their determination. High-resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS GF AAS) is a suitable technique for trace element determination, mainly because of its excellent limits of detection and its extremely high tolerance for complex matrices, favoring also direct solid sample analysis. In this work, the determination of Cu and Mn in infant formulas was investigated using HR-CS GF AAS and direct solid sample analysis. Due to the high content of these elements in the investigated samples, only the central pixel (CP) was chosen for Cu, even when its principal analytical line at 324.754 nm was used. A secondary line, at 403.076 nm (7% of sensitivity) was used for Mn and three pixels (CP±1) were chosen for signal evaluation. Samples were dried, ground in a micro mill and sieved through a mesh of 45 µm. The optimal pyrolysis and atomization temperatures were 1300 °C and 2300 °C for Cu, and 1100 °C and 2100 °C for Mn, respectively. The use of chemical modifiers was not necessary, and aqueous standard solutions were used for calibration. Under these conditions the methods developed allow the direct determination of these elements. The limit of detection (LOD) and the characteristic mass, respectively, were 0.01 µg g⁻¹ and 8 pg for both, Cu and Mn. The limit of quantification (LOQ) was 0.03 µg g⁻¹ for Cu and 0.04 µg g⁻¹ for Mn. The accuracy of the methods was evaluated by the analysis of a rice flour certified reference material (NIST SRM 1568a), and the values found were in agreement with those of the certificate. The concentrations were in the range of 1.3 ± 0.04 and 6.8 ± 0.3 µg g⁻¹ for Cu, and between 0.7 ± 0.1 and 17.2 ± 2.3 µg g⁻¹ for Mn.

Acknowledgment
CAPES and CNPq
By applying a thin (<1 mm) water layer on the top of the machined samples and focusing powerful (energy >50 mJ) femtosecond pulses through a low NA objective, self-focusing and nonlinear absorption phenomena transform the beam to a filament which enables more efficient ablation compared to the conventional focusing in air. It results in superior micromachining quality and throughput due to additional spatial shaping of femtosecond pulses, cooling and cleaning properties of the covering fluid [1]. This method was successfully applied for a fabrication of the complex objects from transparent, semiconductor and metallic samples.

Laser micromachining related with ablation can benefit from laser-induced breakdown spectroscopy (LIBS) as it allows to determine not only the chemical composition, but also can lead to an insight of the instant characteristics or quality of the micromachining. In this report we present results on the application of the LIBS in monitoring of the micromachining of different materials immersed in water with femtosecond high repetition rate pulses. All experiments were carried out using the Yb:KGW laser system with pulse duration 300 fs and power up to 20 W at 1026 nm wavelength, galvanometric scanner and f- theta lens (f = 100 mm). The emission from ablated materials was collected through f- theta lens, scanner and taken away at dielectric mirror used for direction of the laser radiation in similar way as in Ref.2. The investigated samples were soda-lime glass and copper. As can be seen in Figure the LIBS signals from materials immersed in water at pulse energy ~100 mJ are few times weaker than in air, but could be easy resolved and show the same behavior of the emitted lines and some difference in continuum signal. LIBS signal was estimated during the laser processing using various scanning algorithms, speed, pulse repetition rates, pulse energies and its relation to the processing speed was established.

Fig. 1 Emission spectra of copper (left) and soda lime glass (right) samples

References
Laser-Induced Breakdown Spectroscopy (LIBS) is an emerging technique suitable for direct in-situ analysis due to its robustness, instrumental simplicity and multi-elemental capability. Thanks to its advantages, LIBS finds its use in on-line diagnostics of technological processes, e.g. production of biofuels from algae. These applications, however, require increase of measurement stability and repeatability.

Here we present the development and optimization of flat jet nozzle adapted for LIBS analysis of liquid suspensions containing microparticles (wear particles, algae etc.). Presented nozzle is equipped with gas sheath in order to minimize the effect of aerosol which was identified as one of the sources of measurement instability. The nozzle with inner diameter bigger than 1 mm is used as opposed to common nozzles with inner diameter of tens of micrometers. Various gases (air, N₂, He) are tested and crucial design parameters of the nozzle (inner diameter and angle of deflection) are optimized.

Measurements of suspensions performed with the flat nozzle show increase of stability and repeatability. Presented flat nozzle with gas sheath integrated into a LIBS system can be a suitable instrument for analysis of liquids suspensions containing microparticles.

Acknowledgement
The authors gratefully acknowledge the financial support from the project CEITEC CZ.1.05/1.1.00/02.0068 from European Regional Development Fund.
COMBINATION OF LASER-INDUCED BREAKDOWN SPECTROSCOPY AND X-RAY MICRO COMPUTED TOMOGRAPHY FOR HIGH-RESOLUTION ELEMENTAL MAPPING

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Laser-Induced Breakdown Spectroscopy (LIBS) is an established analytical technique that is based on spectroscopic analysis of radiation emitted by a micro-plasma induced on the analyte surface by a laser pulse. The relative simplicity of the LIBS principle makes this technique very attractive for a large variety of applications [1].

X-ray microradiography and micro computed tomography (µCT) techniques were proven as powerful, nondestructive methods capable, for example, of visualizing the sample structure (Fig. 1) before the laser-ablation-based chemical mapping [2].

Here we report on the combination of LIBS and µCT for investigation of biological samples. Special emphasis is given to the demonstration of the possibility to identify different elements and selected nanoparticles in soft tissues by LIBS and a subsequent 3D visualization of the distribution of these elements or nanoparticles using µCT. The advantages and limitations of this approach will be also discussed.

References

Acknowledgment
The authors gratefully acknowledge the financial support from the project CEITEC CZ.1.05/1.1.00/02.0068 from European Regional Development Fund.
OPTIMIZATION OF LIQUID JET SYSTEM FOR LASER-INDUCED BREAKDOWN SPECTROSCOPY ANALYSIS

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Laser-induced breakdown spectroscopy (LIBS) enables direct in-situ analysis of samples in any state of matter [1]. This capability of LIBS enables its utilization in vast variety of applications, for instance bio-applications [2] and online monitoring. We report on the optimization of a jet system for direct elemental analysis of samples in liquid phase using LIBS technique. This system consists of a peristaltic pump and a thin specially designed nozzle producing a thin flow of liquid solution/suspension. Such arrangement was used to reduce splashes of liquid and sedimentation of suspension and thus to improve the repeatability of an experiment.

Firstly, stepping frequency of the peristaltic pump was synchronized with a flashlamp of ablation laser source. Using such synchronization, changes in pressure and hence volume of liquid along the step of the peristaltic pump were mitigated. Changes in the liquid flow volume affect the laser ablation process in the sense of so-called effective volume function [3]. Other phenomenon affecting LIBS signal fluctuations, moving breakdown, was also studied. Afterwards, single pulse (SP; 1064 nm Nd:YAG laser pulse) and double pulse (DP; 1064 nm and 532 nm Nd:YAG laser pulses) LIBS systems were optimized to obtain best possible signal-to-noise ratio. The performance of SP and DP LIBS in detection of heavy metals traces was estimated. As a result, significant improvement in sensitivity in terms of limits of detection using DP LIBS system for analysis of Cu and Pb was observed.

References

Acknowledgement: We hereby acknowledge the founding within the project ‘CEITEC—Central European Institute of Technology’ (CZ.1.05/1.1.00/02.0068).
MULTIVARIATE APPROACH TO STUDY OF ELEMENT ASSOCIATION IN SANDSTONE-HOSTED URANIUM ORES

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This work aims on the description of possible element association within a sample of sandstone-hosted uranium ore by means of laser-induced breakdown spectroscopy (LIBS). The association of elements U-Zr-P-Ti is unique for the ore origin deposit (Břevniště, Czech Republic). According to results of complete chemical analysis of powdered fragments of 26 rocks; a single flat sample, with promising composition, was prepared for LIBS measurement. To achieve best spatial resolution LIBS was employed in the orthogonal double pulse arrangement with spatial resolution of 0.1 mm. It was possible to divide measured dataset into two distinct groups by utilizing artificial neural networks (ANN). One group is associated to the silicon matrix (with major compound SiO₂). Second group can be correlated to the presence of uranium, this means that we can expect aforementioned element association within this group. Presented work shows multivariate analysis, namely principal component analysis (PCA), of non-silicon group in greater detail with focus on describing the elemental lines which provides most variability in data. Such a combination of non-linear and linear multivariate method can lead to better description of the data and ease the discovery of hidden variables and relations.
THE SHREDDERSORT PROJECT: LIBS AND ANN FOR SELECTIVE RECOVERY OF NON-FERROUS METAL AUTOMOTIVE SHREDDER

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This paper reports the preliminary results obtained in the SHREDDERSORT project, a project funded by the European Commission aimed at developing a new dry sorting technology for non-ferrous automotive shredder.

The non-ferrous fractions contain mainly aluminum, magnesium and copper alloys, although sometimes also zinc-based alloys are found. These materials result after the non-ferrous separation (usually by an Eddy-current operation) and can be further sorted by hand-sorting or even by any kind of mechanical sorting process.

The analyses have been realized in the Applied and Laser Spectroscopy Laboratory at CNR in Pisa using the Laser Induced Breakdown Spectroscopy (LIBS) technique, in the perspective of the development of a dedicated instrument for on-line sorting operation.

Different types of samples have been analyzed and, in particular, different parameters have been studied to identify the optimum excitation conditions for the maximization of LIBS signal under double pulse excitation, for instance changing the inter-pulse delays between the laser pulses (from 0ns (coincident pulses) to 75µs) and the laser pulse irradiance.

Finally, the LIBS spectra have been processed using an Artificial Neural Network approach in order to classify different kind of aluminum alloy, using a set of certified samples.
Naturally occurring trace elements play a pivotal role in the function of living organisms. Either present as free ions (e.g., K, Na) or in bound form for example functioning as cofactors for certain proteins (e.g., Cu, Zn, Fe), the portion of metals is a very important part of every cell. Thus, an inequity in the metal balance may indicate abnormal physiological conditions, for example caused by cancer or other illnesses.

Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry (LA-ICP-MS) is well known for its high sensitivity for metallic analytes and the capability of elemental mapping. Using this method, trace elements can be detected and quantified in tissues. Not only naturally occurring elements, but also artificially introduced metals (e.g., platinum from anti-carcinogenic medication) can be detected. Thus, LA-ICP-MS is a well suited tool for medical investigations. Elemental distributions obtained from such chemical analysis can complement results from typically used histological or immunohistochemical investigations. Quantitative analysis can help to describe for example drug uptake mechanisms in closer detail than conventional methods. However, LA-ICP-MS is not capable of analyzing most bulk elements in biological tissues. Hydrogen, nitrogen, and oxygen are inaccessible to this method, while the analysis of carbon is aggravated due to a number of factors. However, also the knowledge about the distribution of these elements might be very valuable for medical questions. In contrast to LA-ICP-MS, Laser Induced Breakdown Spectroscopy (LIBS) can detect all of the mentioned elements with sufficient sensitivity. Conversely, the detection power of LIBS is not high enough to analyze most trace elements in biological tissues. Due to this reason, simultaneous analysis of one sample using LA-ICP-MS and LIBS is necessary: Bulk elements can be detected using LIBS, while trace element distributions are monitored using LA-ICP-MS. Using this so-called Tandem LA/LIBS approach, a complete elemental analysis of tissue samples is possible, opening up new opportunities for advanced elemental imaging of biological samples.

In this work, the capabilities of LA-ICP-MS and Tandem LA/LIBS for the investigation of biological samples are presented. Simple LA-ICP-MS analysis provides accurate quantitative information on trace element distributions, while Tandem LA/LIBS can be employed for complete elemental analysis, if necessary.
ASSESSMENT OF THE MOST EFFECTIVE PART OF ECHELLE LIP SPECTRA FOR CLASSIFICATION PURPOSES; FOR FURTHER USE OF CZERNY-TURNER SPECTROMETER

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Laser-Induced Breakdown Spectroscopy (LIBS) is a popular technique for direct in-situ analysis due to its advantages; such as robustness, instrumental simplicity, multi-elemental detection capability, and in connection with advanced chemometrics techniques also sensitivity and selectivity. LIBS system can be readily employed for stand-off detection in harsh environments, as proved by its presence among other analytical techniques on the Mars Rover, Curiosity.

The advancement of LIBS technique in recent years is influenced by the significant improvement in instrumentation (laser sources, spectrometers and detectors). Conventional LIBS instruments differ according to a designated application when their performance is optimally adapted to reduce namely the costs and turn-around time of analysis. Typically, LIBS analysis provides bulky data sets where each sample spectrum is represented by multivariate information. Thus, more sophisticated utilization of chemometrics results in real-time classification and/or quantification of unknown specimen.

The motivation of this work is driven by the need for improvement in the figures of merit for real-time classification provided by the X-Trace device (AtomTrace) designed for direct stand-off LIBS analysis. Since the radiation of laser-induced plasma (LIP) is collected at a larger distance (i.e. from smaller solid angle) the collected radiation must be analyzed most effectively. Hence the selection of spectrometer is a key attribute of the whole LIBS system. Both essential features (spectral range and optical throughput) of any spectrometer are inversely proportional to each other.

Primary objective of this work is to assess a part of echelle LIP spectra (having working range of wavelengths from 200 to 800 nm) that can be most effectively employed for igneous and sedimentary rocks classification. Obtained spectral windows (given by moving spectral mask of 20 nm width) will be classified using partial least square discriminant analysis (PLS-DA). Afterwards, the Czerny-Turner spectrometer (having higher optical throughput) will be aligned to selected spectral regions and rocks samples will be re-measured. Consequently the PLS-DA analysis will be provided again. Measurements will be done utilizing commercially available Sci-Trace device (AtomTrace), where spectrometers in both configurations (echelle and Czerny-Turner) can be attached to.

Acknowledgment
The authors gratefully acknowledge the financial support from the project CEITEC CZ.1.05/1.1.00/02.0068 from European Regional Development Fund.
Laser-Induced Breakdown Spectroscopy (LIBS) has been widely used in modern analytical chemistry, it shows the growing number of users in different fields of element study from using at cultural heritage, geochemistry, remote sensing, industrial process monitoring, the analysis of bio-samples and recycling to environmental monitoring. This method is so popular because it offers a series of advantages such as fast response, applicability to any type of sample, practically no sample preparation, remote sensing capability, speed of analysis and the main advantage is the possibility of investigation of the elemental spatial distribution.

The use of quantum dots (QDs) as probes for bioanalytical applications is a highly promising technique because fluorescence-based techniques are very sensitive. QDs seem to show the greatest promise as labels for tagging and imaging in biological systems.

In our study suitable procedure for injection of QDs onto a different substrate and optimization of these particles detection using LIBS was focused to achieve the best spatial resolution and the lowest detection limits. Dependence of the LIBS signal intensity on the different parameters was investigated.

The technique described in this poster presentation allows detection of QDs injected on the silica gel spread on aluminum foil or filtration paper. Commercially available table-top LIBS system with software controlled stages in x and y directions was used. The prepared substrates with injected QDs were placed into a lab-made holder. Experimental conditions, as gate delay, gate width, used energy of the laser, volume of applied suspension of QDs and their proper pretreatment and drying were studied.

The feasibility of their 2D distribution mapping on the substrate by LIBS was examined in connection with the separation (or pre concentration) possibilities. Due to the immediate signal response, relatively simply instrumentation and possibility of automation LIBS offers promising and fast alternative to other detection techniques (e.g. fluorescence) because can serve not only for detection of fluorescent QDs but also for nanoparticles which do not show any visible luminescence.

Acknowledgment
Financial support from the project CEITEC CZ.1.05/1.1.00/02.0068 from European Regional Development Fund is highly acknowledged.
IMPROVEMENT OF THE LASER-INDUCED BREAKDOWN SPECTROSCOPY METHOD SENSITIVITY BY COMBINATION OF AG-NANOPARTICLES AND VACUUM CONDITIONS

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Nanoparticles are nowadays used in many different fields. Recent method utilizes the metallic nanoparticles applied on a sample surface to improve the sensitivity of laser-induced breakdown spectroscopy (LIBS) method, so called nanoparticle-enhanced laser-induced breakdown spectroscopy (NE-LIBS). LIBS is atomic emission spectroscopy based method where the laser-induced plasma (LIP) is created by focusing the high energy pulse on a sample surface. LIP emits characteristic radiation corresponding to its elemental composition. To the advantages of this contactless and quasi-destructive method belong fast analysis, measurements of samples in-situ without or with little sample preparation, and simultaneous multi-elemental analysis. Different ambient conditions (vacuum, etc.) affect also the intensity of detected signal. To the limitations of the LIBS method belongs quantitative analysis and low sensitivity in detection of trace elements. There exist several possibilities for enhancement of LIP signal; double-pulse LIBS, LIBS + LIFS (laser-induced fluorescence spectroscopy), NE-LIBS, measurements under vacuum conditions, etc.

In this study we combined the NE-LIBS method and vacuum conditions in order to obtain the highest enhancement in LIP signal, i.e. improvement of the sensitivity. Copper based alloys containing higher number of trace elements (for instance Pb, Al, Fe, Ni, Sb, Sn, As, i.e.) were studied. We focused on the step by step optimization of the measurement parameters, such as energy of laser pulse, temporally resolved detection, ambient pressure, and different concentration of Ag-nanoparticles applied on the sample surface.

Acknowledgment
We acknowledge the support by the project “CEITEC – Central European Institute of Technology” within the framework of the grant STI-S-14-2523 (Advanced Nanotechnologies and Materials).
Bioaccumulation of toxic compounds and elements in living organisms is a major ecological risk. Due to anthropogenic overproduction of these compounds, their concentration in air, water and soil is increasing. Some metals are easily transferred from soil to plants and after that to animals. This study focuses on the accumulation of lead (as a typical toxic heavy metal) in tapeworm Hymenolepis diminuta, caused by the soil-plant-rat-tapeworm lead transport chain. The method of laser ablation with ICP-MS can determine the amount of the toxic elements (e.g. Pb, Cd) and biologically active elements such as Cu and Zn in the tapeworm cross-section samples. Moreover, the technique provides the concentration maps (images) with very good spatial resolution (typically 10 - 100 µm). The results for different body segments of the tapeworm (head, neck, center and the end of the body) are presented and discussed.

Acknowledgement
This project was supported by Czech Science Foundation GA13-18154S, by the project “CEITEC - Central European Institute of Technology” (CZ.1.05/1.1.00/02.0068) from European Regional Development Fund and Student Project Grant at MU (specific research, rector’s programme) - Category A (MUNI/A/1461/2014).
OPTIMIZATION OF LIBS MEASUREMENT PARAMETERS VIA MULTIVARIATE CHEMOMETRICS FOR THE CLASSIFICATION PURPOSE

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The outputs of LIBS analysis are multivariate data sets with several thousand to tens of thousands variables in one spectrum. Such a comprehensive set of information contained in a single spectrum offers a challenge for processing all at once, quickly and efficiently. Multivariate analysis makes it possible by reducing large files of the complex, multivariate data to a smaller number of factors describing the differences between the samples. Chemometrics algorithms have already been applied on LIBS data for classification or quantification purposes.

When focusing on classification, papers published in the past few years confirm the interest in multivariate classification approach. The most used multivariate classification method is principal component analysis (PCA). In these cases, however, only for dimension reduction, since it is an unsupervised technique and is suitable for classification of only simple systems, outlier detection or for preliminary view on the dependencies between the samples in the model. In this work we are primarily aimed on the classification of geo-samples using LIBS and chemometrics, namely PCA, which was already used for this kind of analysis, and support vector machines (SVM).

The key part of classification, however, is the setting of appropriate measurement conditions, because these may differ from conditions used for quantification purposes. The standard procedure is to choose the measurement parameters on the base of signal-to-noise ratio of selected lines. Laser-induced plasma (LIP), however, is very complex in its evolution and emission. That is why we suggest to set the measurement parameters by using overall information which one can get from the spectra. This can be achieved by applying an algorithm, for example PCA. This is the main goal and novelty of presented work, since optimization of measurement parameters for the classification purpose especially has not been solved yet in any previous publication.
DETERMINATION OF CADMIUM AND LEAD IN BIOLOGICAL FLUIDS USING LASER-INDUCED BREAKDOWN SPECTROMETRY

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Cadmium and Pb are toxic metals with probable carcinogenic effect. Trace analysis of these elements in biological fluids with using common spectral methods can be problematic due to matrix effects and related necessity to use a complex time consuming sample preparation techniques. Direct analysis of materials as blood or urine is possible after sample dilution, but such procedure is often connected with significant impairment of limits of detection. Deposition of biological fluids on the solid support and subsequent direct analysis of obtained sample with using methods based on the laser ablation seems to be an interesting alternative. Lowering the minimum sample volume required for analysis, increase in speed of analysis and improved detection limits; they are some of expected advantages of this approach.

Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is the method most commonly used for the analysis of the liquid samples deposited on solid surfaces. Various types of solid carriers and liquid samples with a different matrix were measured. Drying the liquid droplet on the filter paper surface was used in study [1], where Cd, Pb and 11 other elements were determined in water samples [1]. Polystyrene carrier was used in another study [2]. Determination of Cd and Pb in urine was performed within the work of Kumtabtim et. al. [3] Teflon sheets, filter paper, Urine Kid paper and glass slides were used as a carriers in this case. 11 elements in urine deposited on clinical filter paper were determined by Aramendia et. al. [4]. Another method applied for the analysis of liquid samples deposited on solid surface was SS-GFAAS. For example, blood sprayed on the surface of filter was successfully analysed by this method [5].

In our opinion, LIBS is a technique that has the high potential to succeed in analysis of Cd and Pb in biological fluids. Relevant analytes (Cd and Pb) were for example determined by LIBS in phosphate fertilizers in the work of Nunes et. al. [6] LIBS analysis of relevant samples such as cells, microorganisms, animal and plant tissues was performed as well [7]. In work [8] Al, Pb and Sr were determined by LIBS in teeth and bones. Determination of low concentrations of worn metals in oils using LIBS is described in work of Xiu et al. [9].

Based on the results above we assume that the LIBS technique can be used for the determination of Pb and Cd in biological samples such as blood or urine.

References
ELEMENT DETERMINATION IN DIFFERENT SIZE FRACTIONS OF AIRBORNE NANOPARTICLES BY ICPQQQMS

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Particles smaller than ~0.1 μm (called “ultrafine particles” or “nanoparticles”) are especially critical for environment and human health. The typical sources of these nanoparticles are traffic/fuel combustion, biomass burning, geological processes in continental crust, and industrial processes (Goel and Kumar, 2014).

To evaluate the element distribution in these ultrafine particles we used a cascade impactor (Electrical Low Pressure Impactor ELPI+™, Dekati Ltd., Finland) capable separating particles from the range of 6–10,000 nm into 14 particle size fractions. Particulate matter was captured on Whatman® nuclepore track-etched polycarbonate membranes for subsequent element determination. The filters were digested in quartz vessels with HNO3 at a temperature of 250°C for 30 min and a loading pressure of 40 bar Argon using an ultraCLAVEIII (EMLS GmbH, Germany). Samples were transferred and appropriately diluted before element determinations on a triple quadrupole ICPMS (ICPQQQMS, Agilent Technologies, Germany).

Results show clear differences in element distributions among the particle size-fractions. The information allowed the identification of the emission source. Earth crust elements e.g. Ca dominantly occurs primarily in the coarse fraction of particles originating from mechanical processes like abrasion of pavement while other elements e.g. As or S occur in fine particle fractions coming from fuel combustion. In the presentation we discuss the distribution of all 37 elements measured and their impact on human health.

Acknowledgement
The article was elaborated under the support of the project Transport R & D Centre (CZ.1.05/2.1.00/03.0064) and 7AMB15AT009 Direct Determination of Platinum Group Elements in Environmental Samples with Inductively Coupled Plasma Mass Spectrometry

References
NOVEL FULL-LENGTH SELENOPROTEIN STANDARDS FOR QUANTITATIVE PROTEOMICS

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Mass spectrometry is the most powerful technique to study proteomes providing both qualitative and quantitative data. Absolute quantification is more challenging task compared to relative quantification because the standards are required. The optimal strategy in this context is the use of full-length stable isotope labeled proteins as internal standards.

In the presented work, production and characterization of full-length protein standards for human selenoproteins, glutathione peroxidase 3, GPx3, and selenoprotein P, SEPP1 has been demonstrated. These standards will support the development of novel, validated and traceable analytical methods for quantification of human plasma GPx3 and SEPP1.

Protein standard production is achieved by cell-free protein synthesis in \textit{E. coli} extracts. Due to the high reactivity of selenocysteine (Sec) and its very complex \textit{in vivo} incorporation mechanism, in our strategy we produced Sec-free SEPP1 and GPx3 standards. To achieve this, all Sec coding codons (UGA) of coding sequence of SEPP1 and GPx3 proteins were site-mutated to Cys coding codons (UGC). Such prepared vectors were used as DNA templates for cell-free protein synthesis. During protein synthesis $^{76}$Se-enriched selenomethionine ($^{76}$SeMet) was introduced into protein structures allowing for absolute quantification of the newly synthesized full-length proteins by ICP-MS via Se detection (ICP MS tag).

As a proof of concept the produced SEPP1 standard containing $^{76}$SeMet has been applied as internal protein standard for the quantification of natural SEPP1 in certified reference materials and in a real patient sample by species-specific isotope dilution ICP-MS using double affinity HPLC separation.

Acknowledgment
This research was undertaken within HLT05 Metallomics (Metrology for Metalloproteins) of the European Metrology Research Programme (EMRP Researcher Grant). The EMRP is jointly funded by the EMPR participating countries within EURAMET and the European Union.
DETERMINATION OF TOXIC AND ESSENTIAL ELEMENTS IN SEAFOOD BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

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A method for the simultaneous determination of beryllium (Be), arsenic (As), cadmium (Cd), lead (Pb), barium (Ba), thorium (Th), thallium (Tl), vanadium (V), chromium (Cr), manganese (Mn), cobalt (Co), nickel (Ni), copper (Cu), zinc (Zn), and selenium (Se) in the bivalve molluscs species by quadrupole inductively coupled plasma mass spectrometer was developed. Measurements were carried out in the freeze-dried samples after microwave digestion with nitric acid/hydrochloric acid and hydrogen peroxide solution. The whole procedure was fully validated. The internal and external quality controls demonstrated that proposed procedure is reliable for routine analysis of toxic and essential elements in biological samples. Within this methodology concentrations of 15 elements were determined in 85 samples of eight species of bivalve mollusks: dog cockle (Glycymeris glycymeris), Manila clam (Ruditapes philippinarum), Atlantic jackknife clam (Ensis directus), blue mussel (Mytilus edulis), Pacific oyster (Crassostrea gigas), great scallop (Pecten maximus), common cockle (Cardium edule) and hard clam (Mercenaria mercenaria). The samples from five countries were collected on the local warehouses and markets according to the multi-annual monitoring programme “Protection of animal and public health”. The results show the significant site-specific differences in concentrations of Cu, Zn and Pb. Additionally inter-specific differences were found in the concentrations of Cr, Cu, Se, Cd and Ba. Our results have been compared to the maximum levels of toxic elements specified in EU and national regulations. Maximum level of Cd in bivalve molluscs specified in the Commission Regulation (EC) No. 1881/2006 was exceeded in 5% of samples. Although this document doesn’t contain regulations for an arsenic in foodstuffs, many EU countries have established a national action level for this element to enable the interpretation of the monitoring studies. The Polish national action level for As was adopted at 4.0 mg/kg wet weight. This level was exceeded in 16% of samples. High concentrations of As may pose a threat to the consumers health, however to assess the health risk associated with bivalve molluscs consumption, the speciation analysis is necessary.

Acknowledgments
The research was supported by KNOW (Leading National Research Centre) Scientific Consortium “Healthy Animal - Safe Food”, decision of Ministry of Science and Higher Education No. 05-1/KNOW2/2015.
DEVELOPMENT OF THE ETV-O-TOF-ICP-MS TECHNIQUE AND ITS COMPARISON WITH THE O-TOF-ICP-MS TECHNIQUE IN ANALYSIS OF THALLIUM IN SPRUCE NEEDLES

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The major anthropogenic sources of thallium pollution are cement factories and coal power plants. The spruce needles can be used as a bioindicator for monitoring of thallium in the environment. For thallium analysis in the environmental samples, sensitive analytical methods are needed due to its low concentration (e.g. HG / ET-AAS, ICP-MS, ICP-OES, DPASV). The use of electrothermal vaporization (ETV) as an introduction system for inductively coupled plasma mass spectrometry (ETV-ICP-MS) provides an opportunity of ultra-trace analysis of challenging samples such as samples with complex matrix, slurry and solid ones. Another advantage of this method is easier sample preparation [1].

The aim of this study was to develop the slurry sampling ETV-ICP-MS method for thallium analysis in spruce needle samples. Its analytical performance was compared with analysis of mineralized samples using ETV-ICP-MS and classical ICP-MS method. Thallium was determined in samples of spruce needles obtained from several locations in Czech Republic. Spruce needles were cut, dried and cryogenically milled. Then samples were either mineralized with 65% HNO₃ using microwave oven Speedwave MWS-2 (Berghof, Germany) or a slurry was prepared in 0.1% triton X-100. The o-TOF-ICP-MS GBC OptiMass 9500 and ETV unit GF 5000 (both GBC, Australia) were used. The measured thallium isotope was ²⁰⁵Tl. Operational condition of the mass spectrometer and ETV unit were optimized. The optimized pyrolysis and vaporization temperatures were 900 °C and 1650 °C. As a modifier, a mixture of palladium (Pd(NO₃) 4 g.l⁻¹) and citric acid (500 g.l⁻¹) was used for stabilization of analyte at lower temperatures during pyrolysis step and for improve analyte transport efficiency (dosed amount of modifier 8 µl) [1, 2]. The dosed amount of sample for ETV-ICP-MS method was 20 µl. The methods were validated using certified reference materials GBW 10052 and BCR 679. Needle samples were analyzed mineralized (using ICP-MS and ETV-ICP-MS) and in slurry (using ETV-ICP-MS). The LODs of methods were 0.567 (ICP-MS mineralized samples); 0.154 (ETV-ICP-MS mineralized samples) and 0.370 (ETV-ICP-MS slurry) µg.kg⁻¹. Obtained results of ²⁰⁵Tl were 0.0105 ±0.0008 mg.kg⁻¹ for ICP-MS analysis of mineralized samples, 0.0130 ±0.0012 mg.kg⁻¹ forETV-ICP-MS analysis of mineralized samples and 0.0123 ±0.0016 mg.kg⁻¹ for ETV-ICP-MS analysis of slurry samples.

References
HEAVY METALS AND SULFATED ASH TESTING:
AN ALTERNATIVE APPROACH

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The monitoring of inorganic impurities, comprising heavy metals (HM) and sulfated ash (SA) plays a crucial role in the quality control of the pharmaceutical production as some of these may pose significant human health hazards. Inorganic impurities in pharmaceuticals may originate from several sources including starting materials, solvents or reagents, metal catalysts, equipment used throughout the manufacturing process, degradation of packaging material etc.[1].

In this sense, the HM and SA methods employing microwave-assisted digestion with concentrated nitric acid have been developed as alternatives to inappropriate methods recommended by United States Pharmacopoeia (USP) and European Pharmacopoeia (Ph.Eur.). The proposed HM method provides sensitive determination of each USP and Ph.Eur. restricted element (Ag, As, Au, Bi, Cd, Cu, Hg, Mo, Pb, Pd, Pt, Ru, Sb, Sn, V), whereas the SA method allows precise determination of the residual non-volatilized inorganic compounds. Accuracy and precision were evaluated by recovery tests and the HM method was also tested on the limit of detection and linearity in addition. The HM spike recoveries accessed by ICP-MS (Agilent 7700x ICP-MS, Agilent) ranged from 89 to 122 % with a RSD lower than 10 % for almost all USP and Ph.Eur. restricted elements. Similarly, the recoveries of Na2SO4 were closed to 100 % with a RSD below 1.3 % [2].

Finally, both methods were successfully applied for the routine screening of the total content of HM and SA in 12 different active pharmaceutical ingredients coming from the Teva Czech Industries, Ltd. product portfolio. The obtained results were subsequently compared with those accessed by the using dry ashing procedure recommended in USP and Ph.Eur. As expected, the proposed HM and SA methods provide more accurate and precise results in a shorter time and simultaneously reduce the consumption of investigated materials and chemicals as well.

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Acknowledgements
The authors gratefully acknowledge the support from the Ministry of Education, Youth and Sports of the Czech Republic LO 1305.
DEGRADATION OF CHLOROBENZENE COMPOUNDS IN GROUNDWATER BY FERRATE TREATMENT

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Since the chlorobenzenes were widely used solvents in the chemical industry, they are the most frequently detected organic pollutants in groundwater. Their biodegradation is limited therefore their removal needs different technologies based on adsorption or oxidation processes. Our research groups developed an electrochemical way for continuous production of ferrate (FeVI) solution which can be mixed directly with polluted groundwater, in order to oxidize the chlorine-containing compounds.

Our investigations were focused on the degradation of mono-chlorobenzene (MCB), 1,2-dichloro-benzene (1,2-DCB), 1,3-dichlorobenzene (1,3-DCB) and 1,4-dichlorobenzene (1,4-DCB) applying model solutions and real groundwater samples. To determine the concentrations of chlorobenzene compounds before and after treatments a solid-phase – micro-extraction – gas chromatograph – mass spectrometer system (SPME-GC/MS) was used. During the optimization of ferrate treatment the effect of pH, ferrate concentration and the ferrate/CB molar ratios were studied at treatment time of 30 minutes. The highest removal efficiency was achieved at pH 7 in the ferrate concentration range of 10-50 mg/L.

If the model solutions containing the four chlorobenzenes in concentration of 100 µg/L were treated with ferrate in concentration of 50 mg/L, 24, 35, 23 and 19% removal efficiency was achieved for MCB, 1,2-DCB, 1,3-DCB and 1,4-DCB, respectively. In presence of real groundwater matrix these removal efficiency values decreased with 4-9%, because a part of ferrate was consumed by other organic compounds having similar or higher electron donor capacity than the chlorobenzenes.
The two-layered systems Zr(2 mm)-Fe(5 mm) subjected isothermal annealing at 700°C duration to 5 h have been studied by methods of Mossbauer spectroscopy and XRD. The formation of intermetallic phases was revealed. In accordance with hyperfine parameters of spectra these phases were identified as Fe$_2$Zr, Fe$_3$Zr, FeZr$_2$ and FeZr$_3$.

The relative intensities of partial Mossbauer spectra for various phases versus duration of consequent isothermal annealing were presented on Fig. It is evident that there is an intensive phase transformations and on the surface of the matrix α-Fe the ferromagnetic (Fe$_2$Zr, Fe$_3$Zr) and paramagnetic (FeZr$_2$, FeZr$_3$) phases are observed.

The investigations of layered system were performed by method of XRD after each step of thermal annealing. It shows the sequence of phase transformations on the surface of α-Fe from coating side: α-Fe+Zr→FeZr$_3$→FeZr$_2$+Fe$_2$Zr. At that, the reverse side detected reflexes of α-Fe.
MÖSSBAUER STUDY OF MAGNETIC COUPLING AND RELAXATION IN Fe[N(SiPh₂Me)₂]₂ MOLECULAR MAGNET

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Single molecular magnets (SMMs), which are molecules showing stable magnetization of molecular origin [1], are in the focus of the scientific and technological interests. SMMs have potential in the future applications in high-density information storage, quantum computing, spintronics, etc. One of the presently known iron-bearing SMMs is the two coordinate (C-Fe-C) linear molecule Fe[C(SiMe₃)₃]₂, for which an extraordinary high hyperfine magnetic field (higher than 150 T [2,3]) and ferromagnetic coupling [3] were revealed by ⁵⁷Fe Mössbauer spectroscopy. In this work we investigate the two-coordinated Fe[N(SiPh₂Me)₂]₂ complex with the aim to elucidate its magnetic properties, whether or not its molecular geometry and electronic structure leads to the appearance of an extraordinary hyperfine magnetic field at the iron nucleus, and how this field is influenced by the external magnetic field and by the nature of the ligands.

In Fe[N(SiPh₂Me)₂]₂ molecular magnet an extraordinary B = 92 T hyperfine field was found in the 5 K ⁵⁷Fe Mössbauer spectrum under an external magnetic field of 0.1 T. This evidences the presence of an unquenched orbital angular moment at the central iron atom. Fe[N(SiPh₂Me)₂]₂ complex is thus shown to represent a further example of low-coordinate iron complexes where quasi free-ion magnetism visualizes itself through an unquenched orbital moment. Magnetization measurements and hysteresis in magnetization indicated exchange coupling and nanosized magnetic units.

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Acknowledgements
The financial supports from the OTKA (K068135), Czech-Hungarian Intergovernmental Fund No. CZ-11/2007 (MEB040806), LO1305, CZ.1.07/2.3.00/20.0017 and CZ.1.07/2.3.00/20.0058 of the Ministry of Education, Youth and Sports of the Czech Republic grants are acknowledged.
Nuclear and radioactive materials were smuggled across Europe following the break-up of the Soviet Union. Nuclear forensic science was born to examine these materials, and combines techniques of nuclear and material sciences. The most important aim of these investigations is to determine the specific “signatures”, which characterize the given material, and reveal the possible origin of the sample. The Nuclear Security Department at the Hungarian Academy of Sciences, Centre for Energy Research specialized its activity to the analysis of nuclear and other radioactive materials which have been seized in Hungary. The laboratory work, carried out mostly on uranium pellets, consists of physical, radiological, isotope-, elemental, and traditional forensic analysis methods.

Macro- and microscopic examinations are usually performed by optical and scanning electron microscopy (SEM). These methods provide information about the surface, chemical composition, specific features and grain size of the samples which are effective indicators of the production technology. Gamma-spectrometry, as a non-destructive radiological method, helps to determine the activity, gamma-emitter nuclide composition, enrichment and age of the samples.

Besides, several atomic spectroscopic and elemental analytical techniques are also used for forensics purposes like ICP-MS, XRF, PIXE, XRD or ESCA.

Mass spectrometric methods are basic methodologies to identify the origin of the samples. Rare-earth elemental profiles, and other elemental impurities, as well as stable isotope ratios (Pb, Nd, O, Sr) are also high confidence signatures.

In our work several analytical data of origin assessment of the seized nuclear materials and also results from inter-laboratory comparison exercises will be shown. New methods and techniques are also under development to find the relevant signatures.
IDENTIFICATION OF CALCINED ENSIS SILIQUA SHELLS BY X-RAY DIFFRACTION AS A NEW BIOSORBENT TO REMOVE A TEXTILE DYE (DIRECT BLUE 71) FROM AQUEOUS SOLUTIONS

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The textile industry is responsible to produce a large volume of polluted effluents discharging to the receiving environment compared to other industries like food processing, paper and carpet industries [1]. The presence of dyes in effluents causes many damage to the ecological system and creates a lot of disturbance to the groundwater resources [2]. The conventional methods for treating dye-containing wastewaters are coagulation, membrane filtration, precipitation and flocculation but adsorption is considered superior to other techniques because of low cost, availability and ability to treat dyes in more concentrated form[3].

The goal of this research is to develop a new potential biosorbent to remove textile dyes from aqueous solution using calcined Ensis siliqua shells (CESS) waste as a novel and eco-friendly biosorbent which is a very cheap and readily available material in most countries. The identification of CESS was carried out by X-ray diffraction (Philips X’Pert PRO). The biosorption behavior was analyzed based on the Langmuir, Freundlich, Temkin and Dubinin-Radushkevich adsorption isotherms and the results showed that the DB71 followed Freundlich isotherm model. The experimental data of adsorption kinetics were analyzed using the pseudo-first and pseudo-second order kinetic models. Various thermodynamic parameters such as $\Delta G^\circ$, $\Delta H^\circ$ and $\Delta S^\circ$ were calculated indicating that this system was a spontaneous and endothermic process.

Keywords: Direct Blue 71, Calcined Ensis siliqua shells, X-ray diffraction, Biosorption, Kinetics, Isotherms, thermodynamic

References
TOTAL-REFLECTION X-RAY SPECTROMETRY AND CIRCULAR DICHROISM FOR ASSESSMENT OF IN VITRO COPPER TOXICITY INDUCED BY CHELATORS IN HUMAN CANCER CELLS

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Copper is found in all living organism and it plays a pivotal role in mitochondrial respiration, iron absorption, free radical scavenging. In high concentration, Cu is also toxic since it is able of producing reactive oxygen species (ROS), causing lipid peroxidation and directly cleavage of DNA/RNA. Thus, the Cu levels in human organisms are strictly regulated. Several molecules, typically chelators, are known to overcome this strict regulation inducing Cu-dependent toxicity exploited for targeted cancer treatment.

For the present study, HCT-15 and HT-29 colon adenocarcinomas, HT-1080 fibrosarcoma as well as MCF-7, MDA-MB-231 and ZR-75-1 human breast adenocarcinomas were used. As chelators, 2,2'-biquinoline, 8-hydroxiquinoline, APDTC, Dp44mT, dithizone, neocuproine and D(-)- penicillamine were used, the latter as control. Generally, cells were incubated without fetal calf serum by adding 2 μM Cu(II) and chelators in a concentration of either 5 or 50 μM. Metal uptake was studied with total-reflection X-ray fluorescence spectrometry. Evaluation of in vitro cytotoxicity and cytostatic effects of the chelators as well as long time antiproliferative effect were assessed. Independently of the performed experiment, Dp44mT was the most efficient chelating agent. For the rest of the investigated compounds, the following toxicity order could be established: neocuproine > APDTC > 8-hydroxyquinoline > dithizone > 2,2' biquinoline, whereas D(-)-penicillamine did not show any toxicity. The IC₅₀ values decreased considerably in the presence of Cu. As in the case of cytotoxicity, a similar tendency could be observed for cytostatis. The colony forming ceased at the 6-h-long treatment for Dp44mT, whereas the decrease in colony forming, and consequently cytostatic activity, was observed for the rest of the Cu chelating agents only at the 24-h-long treatment. Elevated Cu concentration (from 0.5 μM to 50 μM) caused higher apoptotic cell ratios in combination with Dp44mT and 8-hydroxiquinoline already after 20 min. Thus, the key to explain the toxicity mechanism of Dp44mT should be connected to the intracellular binding of Cu ions. Each investigated chelator induced ROS generation in the presence of Cu(II). Circular dichroism spectra demonstrated that the investigated chelators - except for neocuproine – restored DNA damage induced by free Cu(II).
THEORETICAL AND EXPERIMENTAL INVESTIGATION OF ANIONIC AFFINITY OF TWEEZER TYPE RECEPTOR

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Hydrazone functional group is known to bind anions due to the presence of acidic N-H group, which potentially interact with negatively charged anion. In order to introduce selectivity for an anion of interest, the hydrazone functional can be introduced in a suitable cavity to allow anion of particular size or geometry to form hydrogen bond with N-H group. To achieve a strong optical signal, the nitro groups can be introduced in the receptor. Therefore, tweezer type receptors with hydrazone and multiple nitro groups were developed by constructing them around α-phthalaldehyde as the spacer. The synthesized receptors were characterized using 1H, 13C-NMR, HR-MS, Elemental analysis and single crystal X-ray crystallography. The Single crystal X-Ray studies revealed temperature dependent polymorphism. The receptor molecule crystallized in P(-1) space group at 100K while at 25°C, the receptor crystallized in P2₁ space group. The crystal structure at room temperature revealed the formation of exclusion and inclusion complex between the receptor molecule and the DMSO while only exclusion complexes are observed in the crystal structure obtained at 100K. The polymorphic crystal revealed that the DMSO molecules are held to the receptor through H-bonds. Several short intramolecular and intermolecular contacts were also observed in the crystal packing diagram. The receptors were first evaluated for affinity towards anions through naked eye detection followed by UV-Visible spectroscopy. The naked eye detection of anions revealed the formation of dark red color change visible to naked eye in the presence of one equivalent cyanide ion, while no color change was observed in the presence of other anions. During the complex formation, the cyanide ion displaced the DMSO molecule present in the cavity of the receptor with the development of dark red color. The UV-visible spectroscopy studies suggested the appearance of a new absorption band at 550 nm in presence of one equivalent cyanide ion. No change in color or absorption spectra was observed in the presence of other anions. The complex stoichiometry was determined through Job’s plot method, which suggested it to be 1:1. NMR spectroscopy was used to study the mechanism of complex formation and DFT calculations confirmed the interactions between cyanide ion and the receptor molecule.
APPLICATION OF A NOVEL DERIVATIZATION TECHNIQUE FOR GLYPHOSATE AND AMINOMETHYLPHOSPHONIC ACID ANALYSIS BY GAS CHROMATOGRAPHY - MASS SPECTROMETRY

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The continued and excessive application of chemicals in agriculture is one of the main causes of the increased environmental pollution which threatens the human wellbeing. One such herbicide which has a steadily increasing use in the agriculture is N-(phosphonomethyl)-glycine (Glyphosate, GLYP) with a major degradation product, aminomethylphosphonic acid (AMPA).

So far, GLYP and AMPA, has been analysed using rapid, simultaneous and reliable detection techniques, including methods, such as gas chromatography- mass spectrometry (GC-MS), in which a preliminary derivatization step was required in order to increase volatility of the compound [1]. With the application of N-methyl-N-(trimethylsilyl) trifluoroacetamide (MSTFA) reagent, resulting in trimethylsilyl (TMS) derivatization - followed by gas chromatography mass spectrometry (GC-MS), a new method for GLYP and AMPA determination is developed. This method introduces a previously unrecognized formation of the AMPA.4TMS (m/z 453), and the GLYP.5TMS (m/z 529) where the reaction shifts GLYP’s equilibrium to be a five active protons containing C=C(OH)2 moiety. In order to fully recognize this development, Density Functional Theory (DFT) modelling was used and by calculating the relative energy values for optimized structures, the formation of stable tautomer structure, GLYP.5TMS was proved.

The optimum conditions were accepted as heating the derivatization solution at 80 °C for 30 minutes. The composition of the solvents used has affected the formed product characteristics and the distribution. Acetonitrile (ACN) and ethyl acetate (ETAC), both which have acidic nature have favoured the AMPA.4TMS formation. For GLYP, however where ETAC favours the GLYP.4TMS, ACN favours the GLYP.5TMS formation. In regards to this, MSTFA/ACN composition was chosen for the simultaneous quantification of GLYP and AMPA. This allowed for detection at and below 1 ng for GLYP.4TMS+GLYP.5TMS and AMPA.4TMS.

Simultaneous quantification of GLYP and AMPA in several different matrices, also increases the practical application possibilities as seen with the impurity analysis of herbicide market samples; average of 4.08 RSD% and 3.42 RSD%, respectively where the nominal and found values are between -15% and -2.9% for GLYP.

A new and reliable method for quantitative analysis of the GLYP and AMPA with alkylsilyl derivatization followed by GC-MS is established. The use MSTFA derivatization of GLYP and AMPA is observed to allow for formation of the fully trimethylsilylated AMPA (AMPA.4TMS) and GLYP derivatives (GLYP.4TMS and GLYP.5TMS). The application of MSTFA/ACN shows a promising improvement for the practical utility of the TMS derivatization, assisting in the analysis of the agrochemical compounds [2].

References


Microwave assisted chemical bath deposition (MW-CBD) method has attracted attention in fabrication of Nitrogen (N) doped ZnO nanostructures. The MW-CBD method was used to prepare nanostructure N doped ZnO films onto silicon (Si) substrates. Zinc nitrate hexahydrate, Ammonium nitrate and an equal molar concentration of hexamethylenetetramine were dissolved in DI water. The solution was stirred 2 h at 90 °C. After, solution was irradiated using a temperature-controlled microwave synthesis system at 600 W and 10 min irradiation time. The films were washed with DI water to remove the remaining salt. Finally, the films were dried at 60°C for 1 h. The effect of N content on the structural, morphological and optical properties of ZnO films was investigated. To investigate the crystalline structure and the orientation of the films, XRD patterns were used. The lattice parameters and texture coefficient values of the films were determined. The important changes in crystalline structure of the ZnO films were observed due to the N content. Field emission scanning electron microscope (FESEM) was used to analyze the surface morphology of the ZnO films (Figure 1). The reflectance values converted to absorbance by application of the Kubelka–Munk function were used to determine the value of optical band gap of the films.

Figure 1. FESEM photography of the films

Acknowledgements
This work was supported by Anadolu University Commission of Scientific Research Projects under Grant No. 1305F082 and 1402F055.
PHYSICAL PROPERTIES OF BORON DOPED NANOSTRUCTURE ZnO FILMS ONTO QUARTZ SUBSTRATE

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Owing to its wide band gap characteristic, transparent conducting zinc oxide (ZnO) films have attracted a lot of attention for a variety of potential applications in both microelectronic and optoelectronic devices such as solar cell, transparent conducting electrode, UV and blue light emitter and thin film transistor. In this study, undoped and boron (B) doped nanostructure ZnO films were prepared by sol gel spin coating method onto quartz substrate. Zinc acetate dihydrate \([\text{Zn(CH}_3\text{COO)}_2\cdot2\text{H}_2\text{O}\text{]} (\text{ZnAc})\) was used as a starting material. 2-methoxethanol \((\text{C}_3\text{H}_8\text{O}_2\text{)}\) and ethanolamine \([\text{C}_2\text{H}_7\text{NO}\text{]} \text{(MEA)}\) were used as a solvent and stabilizer. The dopant source of boron came from trimethyl borate \([\text{(B(OCH}_3\text{)}_3\text{]} \text{(TMB)}\). XRD experiments were performed in air with a laboratory X-ray powder diffractometer at room temperature. The ZnO film was found to be polycrystalline with a (002) preferred orientation. Secondary peaks detected were (100) and (101). It was further found that incorporation boron resulted in decrease in the intensity of the (002) peak. The surface morphological features of the films were analyzed using FESEM. Atomic force microscope (AFM) images were assessed over a 1x1 mm area by non-contact mode. AFM images of the surface morphology are shown in Fig. 1 for undoped and B doped ZnO films. The films have very high optical transmission in the visible range (400–800 nm). The average values of transmittance are about 85%.

Acknowledgements
This work was supported by Anadolu University Commission of Scientific Research Projects under Grant No. 1305F082.

Figure 1. AFM images of the the undoped and B doped ZnO films
INVESTIGATION OF THE LONG-TERM EFFECTS OF METAL POLLUTION IN TISZA RIVER BY SEQUENTIAL EXTRACTION

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The Hungarian section of the Tisza River is highly influenced by metal pollution sourced from mining activity in Romania. Mining in Maramures County (former Máramaros) traditionally exploits ores of base metals (Cu, Zn and Pb) and precious metals (Au and Ag). Besides, metal pollution has also a long history in the upper Tisza catchment. Nowadays, the processing of old tailings pond material by using cyanide to recover Ag and Au is spreading in this region. Mining activities that use dangerous and toxic chemicals such as cyanide can be serious sources of contamination. Besides, wastewater may contain heavy metals associated with fine-grained sediments. However, metal concentration of river water is not remarkable 30 km downstream from the point sources, sediment-associated metals are dispersed much greater distances.

In January and March 2000 two tailings dam failures occurred in Baia Mare (Nagybánya) and Baia Borsa (Borsabánya) and resulted cyanide and metal pollution in the Lápos - Szamos - Tisza and metal pollution in the Visó - Tisza river systems, respectively. The short term effects of the pollution events were studied by many researchers, and water and sediment of the Lápos-Szamos-Tisza and Visó-Tisza riversystems were found to be contaminated by Cu, Zn, Pb and Cd.

The mining accidents were followed by floods; therefore the metal pollution of the floodplains was also observable. Deposition of contaminated sediment on floodplains during flood events and the mobilization of the pollutants may increase the plant available metal content of the upper soil layer. The mobility and phytoavailability of metals depend on their chemical forms. Therefore, it is appropriate to examine the amount of the elements by sequential extraction procedures (SEP).

Considering the above information it is likely that the residual heavy metal load may entail economic effects that cannot be envisaged at the moment as the Tisza river valley is under agricultural use (pastures, meadows, orchards, arable crops). This is the reason why intensive research has been started aiming at testing and monitoring the ecological systems of both water and floodplains.

The aim of this study was to evaluate the term effects of these pollutions on the total and phytoavailable metal content of soils of samples collected in 2000 and 2013 from floodplains and pastures along the Tisza (Tivadar, Vásárosnamény, Rakamaz, Tiszacsege) and comparing these results to our earlier ones.

Acknowledgement
This research was supported by projects: Hungarian Science Research Fund (OTKA 108558).
Laser Ablation (LA) in conjunction with inductively coupled plasma mass spectrometry (ICP-MS) method is widely used in many branches of modern analytical chemistry. These direct analyses allow obtaining the elemental composition of the samples. The chemical composition of the formed aerosol and the particle size distribution are important parameters responsible for the successful quantification analysis. The properties of the particles depend primarily on the parameters of the laser beam and the sample type.

This work deals with online monitoring of the aerosol generated by nanosecond ArF laser ablation system at the wavelength of 193 nm using a particle analyzer FMPS (Fast Mobility Particle Sizer) and SMPS (Scanning Mobility Particle Sizer). Pressed powdered tablets of standard reference material GBW 03101 were compared to varying ratio with a wax as a binder. LA-ICP-MS signal was also investigated. The suitability of wax as a binder for pressed powders is discussed.

Acknowledgements
The authors acknowledge the European Regional Development Fund project “CEITEC - Central European Institute of Technology” (CZ.1.05/1.1.00/02.0068) and Project Grant at MU MUNI/A/1461/2014 from program Specific research and grant P503/12/G147. This work was also financed from the European Social Fund, Project CZ.1.07/2.3.00/30,0034.
The doped zinc oxide (ZnO) films have attracted much attention because of their great potential for application to transparent conducting electrodes and insulating or ferroelectric layers in optoelectronic devices. Therefore, the structural, optical and electrical properties of the doped ZnO films have attracted great interest. In this study, ZnO and ZnO:Al films were deposited onto glass substrates by the sol gel method using spin coating technique. The effects of Al dopant on the crystalline structure and orientation of the ZnO films have been investigated by X-ray diffraction (XRD) study. X-ray diffraction patterns confirm that the films have polycrystalline nature. ZnO and ZnO:Al films have (0 0 2) as the preferred orientation. This (0 0 2) preferred orientation is due to the minimal surface energy which the hexagonal structure, c-plane to the ZnO crystallites, corresponds to the densest packed plane. Optical transmittance and reflectance of the films were recorded with a double beam Shimadzu UV 2450 spectrophotometer with an integrating sphere in the wavelength range 190–900 nm. The optical absorption study reveals that the films have a direct band gap. The optical constants of these films, such as refractive index, extinction coefficient, optical dielectric constants and optical conductivity were determined using transmittance and reflectance spectra.

Acknowledgement
This work was supported by Anadolu University Commission of Scientific Research Project under Grant No. 1305F082.
QUANTIFICATION OF RARE EARTH ELEMENTS RETAINED ON NATURAL BIO-PARTICLES COVERED WITH IONIC LIQUID IN COMBINATION WITH ETV-ICP-OES

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Rare earth element (REE) are present as impurities in phosphate fertilizers used in agriculture, and might enter the human food-chain, as they are taken up by plants. To analyze REEs in chemically digested plant material, inductively coupled plasma optical emission spectrometry (ICP-OES) is used. However, determination of REEs by ICP-OES needs enrichment prior to analysis due to their low concentration.

In this work, an innovative approach is presented, which is based on preliminary enrichment of REE using dispersed particle extraction (DPE), followed by sensitive measurement by means of electro thermal vaporization (ETV) coupled to ICP-OES. In DPE, adsorbent particles are dispersed in the sample solution, after a reaction time of few minutes the supernatant is separated from the analyte containing sorbent particles. The applied adsorbent is a natural bio particle, Lycopodium clavatum spore, with the size of 30 ± 4 µm and high porosity. This bio particles were covered by an ionic liquid salt [P6614][BEHPA] which acts as the ion exchanger and extracts REE ions from the sample digest.

For element specific analysis, the precipitated particles are transferred into a graphite boat and measured using ETV-ICP-OES, which allows an efficient separation of the organic sorbent matrix and thus a measurement of REE without spectral interferences. Using the inexpensive nature-made particles with easily tunable ionic liquids for analyte-enrichment in combination with ETV-ICP-OES analysis has been found to provide satisfying sensitivity in the analytical context presented here, as well as good reproducibility.
DEPOSITION AND CHARACTERIZATION OF SOL GEL COATED ZnO FILMS: AS A FUNCTION OF SOL MOLARITY

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Zinc oxide is a direct, wide bandgap (3.37 eV) semiconductor material with many promising properties for optoelectronics, transparent electronics, spintronic devices and sensor applications. ZnO has numerous attractive characteristics for electronics and optoelectronics devices. The exciton binding energy is ~60 meV for ZnO, The room temperature electron Hall mobility in single crystal ZnO is ~200 cm² V⁻¹. ZnO can be grown on inexpensive substrate, such as glass, at relatively low temperatures. ZnO has a hexagonal wurtzite crystal structure, with lattice parameters a=3.25 Å and c=5.12 Å [1].

ZnO films have been prepared by a variety of deposition techniques such as chemical vapour deposition, sputtering, spray pyrolysis, and sol-gel method, etc. Among the preparation methods of ZnO films, sol-gel is an excellent method [2]. Coating of substrates by the sol-gel method is very useful for modifying properties of substrates with a large or small surface area or providing substrates with new active properties, which are needed for developing optical, electronic and chemical devices [3].

In this study, ZnO films have been deposited by sol-gel dip coating method. The concentrations of ZnAc solution were adjusted as 0.25, 0.35, 0.45 and 0.55 M. Substrate was dipped at withdrawn speed of 6 mm/min. X-ray diffraction (XRD) results were analyzed to understand the effect of sol concentration on the crystalline structure and orientation of the films. The films exhibited (002) preferred orientation. The surface microstructure of films were investigated for using field emission scanning electron microscopy (FESEM). The electrical transport characteristics (hall mobility and electron concentration) were investigated by a Hall measurement system using the Van der Pauw configuration under 0.55 T magnetic field at room temperature.

References

Acknowledgement
This work was supported by Anadolu University Commission of Scientific Research Project under Grant No. 1305F082.
OPTIMIZATION OF MICROWAVE-ASSISTED EXTRACTION FOR FLY ASH ELEMENTAL COMPOSITION DETERMINATION BY oaTOF-ICP-MS

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In this work a novel, simple, efficient and environmentally friendly microwave-assisted extraction (MAE) method using ammonium fluoride as the extractant prior to multi-elemental analysis of fly ash samples by inductively coupled plasma orthogonal acceleration time-of-flight mass spectrometry (oaTOF-ICP-MS) was developed. This method avoids handling the corrosive and/or toxic acids like HF, HCl or HClO₄ being commonly used during sample preparation of the fly ash samples. Thus, it prevents the potential risk of analyte loss due to the creation of volatile fluorides and eliminates the formation of different polyatomic species interfering the determination of number of elements during the oaTOF-ICP-MS analysis. The optimum extraction parameters evaluated using a fractional factorial design were as follows: 10 mg of the sample extracted with 5 mL of 140 g L⁻¹ NH₄F for 10 min at 200 °C. The optimized MAE procedure was successfully applied to the determination of 11 elements (Li, Be, Ni, As, Se, Rb, Sb, Cs, W, Tl and U) in two certified reference materials, namely Fine Fly Ash CTA-FFA-1 and Constituent Elements in Coal Fly Ash Standard Reference Material® 1633b. The obtained results were in a good agreement with the certified or comparative values with an overall precision better than 10% in all cases.

Acknowledgement
Financial support from the University of Pardubice (project no. SGFChT_2015001) is gratefully acknowledged.
COMPARATIVE STUDY OF EXTRACTION METHODS APPLIED FOR ESTIMATION OF BIOLOGICALLY AVAILABLE FRACTIONS OF POTENTIALLY TOXIC ELEMENT (PTE) CONTENT OF SOILS AND SEDIMENTS

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In this study the efficiency of different standardised and recommended extraction procedures was compared using soil samples of different physical characteristics. The batch leaching methods were applied using the following extraction reagents: distilled water [1], CaCl₂ – DTPA [2], KCl – EDTA [3] and Lakanen Erviö [4]. The information content of these methods was compared with the BCR recommended sequential extraction procedure and for the determination of pseudo total soluble element content the HNO₃/H₂O₂ in microwave digestion was applied [1].

The BCR methodology simultaneously provides much more information about the chemical forms and mobility of PTEs as the batch leaching techniques [5].

For element detection in different extraction solutions a multielemental ICP–OES methodology was applied with matrix matched calibration.

On the basis of our results it can be established that the soluble element content is strongly influenced by the physical types of soil, and in batch leaching techniques the EDTA-complexing is the most effective. By the BCR sequential extraction method in the extraction step similar amounts of PTEs can released as by the complexing-agent batch leaching. The reliability of the spectrochemical element detection is influenced by matrix effects caused by the extractant media therefore the reliable comparison required a careful calibration and validation for all extractant media.

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Acknowledgement
This research was supported by Hungarian Science Research Fund (OTKA 108558).
Sample digestion is an important procedure and directly affects on the reliability of quantitative analysis of total selenium in Se-enriched yeast products. The home-digestion closed digestion system was successfully developed by specially designing and constructing from the basic equipments in laboratory that consisted of 4 main devices; water bath, cover plate, vessels and wind tunnel. The optimum conditions of the home-made closed digestion system was accurately and precisely achieved by using 2.0 ml of nitric acid for 0.1 g Se-enriched yeast sample, 100 °C digestion temperature and 20 min digestion time. These conditions showed good validation and acceptation with the certified value of Se-enriched yeast reference material. Furthermore, the digestion efficiency of home-made closed digestion system was as as the recognized digestion methods especially microwave assisted digestion. Consequently, the home-made closed digestion system could be efficiently utilized as an alternative digestion method for total Se determination in Se-enriched yeast products. Additionally, the home-made closed digestion system was adapted from a basic instrument in laboratory which has affordability and easier operation rather than the recognized methods.

Keywords: ICP-MS, closed-digestion system, Se-enriched yeast

References
DETERMINATION OF BROMINE IN SELECTED POLYMER MATERIALS AND PRINTED CIRCUIT BOARDS (PCB) USING DIFFERENT ANALYTICAL METHODS

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European Community Directive 2002/95/EC (also known as the RoHS directive) restricts the use of the selected hazardous substances in electrical and electronic equipment. One of the restricted elements is bromine. RoHS limits its use in the form of polybrominated biphenyls (PBB) and polybrominated diphenyl ethers (PBDE) fire retardants in components of electronics and electrical goods. Target level in a given homogeneous material found in a product component should be lower than 1000 ppm for Br (in PBB and PDBE). X-ray fluorescence spectrometry (XRF) is a convenient and suggested method for detecting the presence and determination of bromine in those materials [1].

In this work, different quantitative methods were studied for the determination of bromine in polymer materials and PCBs from wasted personal computers and mobile phones. Prior to analysis, crushed samples were decomposed by combustion in a high-pressure container after applying an oxygen partial pressure of 30 bar. Combusted gas was absorbed in sodium hydroxide solution (0.2 mol/L).

Total bromine concentration was determined in obtained solutions using NexION 300D inductively coupled plasma mass spectrometer ICP-MS (PerkinElmer) with internal standardization (Y, 10 µg·L⁻¹), in linear dynamic range of calibration curve from 0.1 mg·L⁻¹ to 10 mg·L⁻¹, (concentration in solid sample: 0.001 % to 25 % w/w).

Bromide (as Br⁻) concentration was also determined by Ion-Selective Electrode method (ISE) and titration methods (argentometry potentiometric titration and iodometric titration).

The results obtained with different quantitative methods shows good agreement with the values obtained by the reference method - XRF.

The accuracy of the methods was tested by analyzing certified reference materials for polyethylene (LDPE): ERM-EC680K (0.0092%-0.010% Br) and ERM-EC681K (0.073%-0.081% Br). The obtained results were consistent with certified values.

Reference
[1] EN 62321-3-1:2013 Determination of certain substances in electrotechnical products - Part 3-1: Screening - Lead, mercury, cadmium, total chromium and total bromine by X-ray fluorescence spectrometry
A SIMPLE AND FAST METHOD FOR PREPARATION OF FISH OIL SAMPLES FOR THE DETERMINATION OF CADMIUM AND CHROMIUM BY HR-CS GF AAS

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Fish are the most common source of OMEGA-3 in human diet [1]. However, fishes are a vehicle of exposure to high concentrations of heavy metals due the biomagnification effect [2]. The value of heavy metals in fish meat is a concern.

One of the most dangerous contaminants in sea food is cadmium [3] and pointed as a Group-1 carcinogen [4]. The trivalent chromium is an essential trace element for humans, since it regulates the fat metabolism and natural glucose [5]. The fish oil capsules are an alternative to have the benefits of the fish meat without the risk of contaminations by heavy metals. The general process of obtaining the OMEGA-3 involves extraction from raw material and refining steps, needed to remove the toxic compounds, such as heavy metals and pesticides [1].

This work proposes a method to determine the chromium and cadmium content at trace levels by high-resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS GF AAS) present in raw and processed fish oil, with a simple and fast sample preparation step: approximately 1 g of fish oil is filled up to 5 mL with 1-propanol. The samples are homogenized manually and injected into a graphite tube with a PIN platform, treated with platinum as a permanent chemical modifier for cadmium determination or without modifier for chromium determination. Palladium was also used as chemical modifier in solution for cadmium determination. The pyrolysis/atomization temperatures were fixed at 1000 °C / 1700 °C for cadmium and 1100 °C / 2400 °C for chromium. The method was applied to fish oil, cocoa butter and milk butter. The limits of detection and quantification for cadmium were 0.5 pg and 1.5 pg respectively, and 7 pg and 23 pg, respectively, for chromium. The accuracy of the method was verified comparing the proposed method with the results obtained after microwave-assisted digestion. Both methods showed no statistical difference, based on a t-student test with a confidence level of 95%.

References

Acknowledgment:
CNPq, INCT E&A
We recently synthesized naturalized dyes (NDs) which are a new class of environmentally friendly chemicals. NDs can be obtained by the covalent union of a dye species (e.g., azo, anthraquinone, aniline type chromophore) with lactose, a natural sugar. In the present work, NDs and the traditional acid dyes (ADs) were compared by studying the different behavior during the leather dyeing processes. NDs are able to confer water-soluble properties to the dye molecule as a whole. The interactions between the dyes and the leather proteins were studied by FT-IR spectroscopy and thermogravimetric (TG) analyses. The protein cross-linking of the dyed leather samples was investigated by studying the 1654/1690 cm⁻¹ peak height ratio and a deconvolution procedure of the amide I peak. The helix secondary structure was the predominant component of the leather proteins of the samples dyed with low concentrations of NDs (2%), while the β-sheets prevailed when leather samples were dyed with the traditional ADs and high concentrations of NDs (>5%). The data were discussed with respect to TG results.

Acknowledgements
This work has been financially supported by the European Project Life+ 2012 ENV/IT/352-“BIONAD”.

References
PHOTOCHEMICAL VAPOR GENERATION OF INORGANIC SELENIUM SPECIES AT TRACE LEVEL WITH GERMICIDAL AND MICROWAVE UV LAMPS

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Nowadays photochemical vapor generation (photo-CVG) is a good competitor of conventional chemical vapor generation for the determination of hydride-forming elements, transition metals and non-metals. Photo-CVG is based on absorption of ultraviolet (UV) radiation by a low molecular weight organic acid, which generates radicals necessary to the vapor generation process [1, 2].

Our study is focused on the application of this technique to Se(IV) and Se(VI) inorganic species. Using a commercial UV germicidal lamp and formic acid at low concentrations, we obtained Se(IV) yields comparable to those of the classic CVG methods. Se(VI), instead, was much less efficient, with yields at least 12 times lower respect to Se(IV), but, unlike hydride generation, still detectable at trace level.

Se(IV) photo-CVG at low acid concentration was tested with several inorganic interferences commonly present in real or digested matrices. We found nitrate ion enhanced selenium vapor photo-generation in a very short concentration range, with experimental trend similar to that of iodine, while Cu(II) resulted the most interfering metal cation.

In our work, we also aimed to extend the operating range of the photo-CVG from usual commercial electroded lamps to mercury microwave-electrodeless discharge lamps (MW-EDL). To the best of our knowledge, this type of UV lamps has been employed for organic matter pre-digestion process [3] and for the photo-CVG of Hg for trace analysis[4]. Here it is reported for the first time the generation of volatile derivatives of Se(IV) species by using photo-CVG with MW-EDL prototypes.

Data collected from mercury-MW/UV photo-CVG analysis have shown behaviors similar to those of electroded UV lamp and yields depending on microwave generator power. Photo-CVG experiments made with this “mercury-filled” lamp (main emission spectral lines at 254 nm) was compared to an homemade cadmium MW-EDL (main emission spectral line at 228 nm) in order to evaluate the photochemical efficiency based on different ultraviolet spectral lines.

References
SEPARATION, PRECONCENTRATION AND DETERMINATION OF MERCURY IN ENVIRONMENTAL SAMPLES BY USING WATER EXCHANGEABLE LIQUID LIQUID MICROEXTRACTION AS GREEN EXTRACTION METHOD COUPLE WITH COLD VAPOR TECHNIQUE

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This study was conducted on a green analytical separation method for determination of mercury from solid matrices. The proposed method of exchangeable water based on liquid-liquid microextraction (EW-LLME) was introduced as a separation method. Exchangeable water (EW) was made by the reaction of carbon dioxide (CO₂) with diethylenetriamine (DETA). Reversible exchanging of the aqueous medium from homogenous EW and polar organic solvent to heterogeneous phase separation by exposed to CO₂. The advantage of CO₂ as compared to other, it is inexpensive, non-hazardous, non-accumulation, easily removed and not requires the transparent material. The exchanging phenomena of EW from low polarity to high polarity were confirmed by FTIR spectrophotometer. The complex formation between Hg and 1,5-diphenylcarbazone was achieved under the optimized experimental conditions. Validation of the EW-LLME method was checked by using certified reference materials and the results were found to be in good agreement with the certified values. The enhancement factors and limits of detection of the proposed method were obtained to be 45.2 and 0.5 ng L⁻¹, respectively. The desired EW-LLME method was successfully applied for the determination of Hg in environmental samples.

Acknowledgments
Jamshed Ali is grateful to the Scientific and Technological Research Council of Turkey (TUBITAK) for awarding him “2216 Research Fellowship Program for Foreign Citizens” and providing financial support. Dr. Mustafa Tuzen thanks to Turkish Academy of Sciences for financial support.
SWITCHABLE SOLID LIQUID DISPERSIVE MICROEXTRACTION OF SELENIUM ON MWCNTS AND GFAAS DETERMINATION OF IT IN WATER SAMPLES

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Dispersive solid phase extraction is reliable and efficient method for analytical processes. Dispersive solid phase extraction is one of the most convenient and promising sample preparation approaches.

A simple switchable hydrophobic–hydrophilic transition of multiwall carbon nanotube (SMWCNTS) has been used as dispersive/extractive medium for selenium from real samples by the stimulation of CO₂. Tetraethylenepentamine (TEPA) functionalized multiwalled carbon nanotubes (MWCNTs) were synthesized and employed as the adsorbent for determination of total inorganic selenium by dispersive solid-liquid microextraction (DSLME) coupled graphite furnace atomic absorption spectrometry (GFAAS). The switching phenomena of functionalized MWCNTs from hydrophobic to hydrophilic were confirmed by FTIR and SEM. Various analytical parameters were optimized. Enhancement factors (EF) and limit of detection (LOD) were obtained to be 72 and 0.015 µg L⁻¹, respectively for selenium. Validation of the developed method was carried out using a certified reference material. The proposed method was successfully applied for determination of selenium in water samples.

References

Acknowledgments
Naemullah is grateful to the Scientific and Technological Research Council of Turkey (TUBITAK) for awarding him “2216 Research Fellowship Program for Foreign Citizens” and providing financial support. Dr. Mustafa Tuzen thanks to Turkish Academy of Sciences for financial support.
The aim of this research was to study the processes of biotransformation of selenium in plant samples: garlic, radish sprouts and sunflower sprouts using mass spectrometry methods. First step included preparation of the research material for quantitative analysis (microwave-assisted digestion) and speciation analysis (extraction with enzymatic hydrolysis).

The first step of the study included determination of total selenium content in the research material with the use of inductively coupled plasma mass spectrometry method (ICP-MS) and monitoring $^{82}\text{Se}$. In a further step speciation analysis of selenium in extracts from biological samples was performed. Coupling ICPMS as detection method with high performance liquid chromatography (HPLC-ICP-MS) as compounds separation method allowed for identification of Se compounds by matching the retention times of sample compounds with standards. In this way Se-methylselenocysteine, selenomethionine, $\gamma$-glutamyl-Se-methylselenocysteine and inorganic $\text{SeO}_3^{2-}$ were identified in the analyzed plant extracts. However registered chromatograms included additional $^{82}\text{Se}$ signals which couldn’t be identified due to the lack of standards.

Qualitative analysis of unknown compounds was achieved using high-resolution mass spectrometer equipped with mass analyzer Orbitrap coupled to ultra performance liquid chromatography (UPLC-MS/MS). Since selenium has six stable isotopes of different abundance in nature, mass spectra of selenium compounds contain very characteristic isotopic pattern. In order to elucidate the structure of unknown Se compounds, selected compounds are subjected to the fragmentation in the collision cell. Structure of unknown compound was determined on the basis of its fragment ions. That allowed for the identification of selenomethionine oxide, 2,3 dihydroxypyridine - selenocysteine, 2,3 dihydroxy-propionylselenoalanthionine, 5’selenoadenosine, selenohomolanthionine and N-acetylcysteine-selenohomocysteine.

Acknowledgements

Financial support from National Centre of Science (NCN, Poland), for the project „Investigation of chemical and biological processes of selenium biotransformation in selenophilic plants and probiotic bacteria towards their application as functional food”, 2012/05/B/ST4/01219 is gratefully acknowledged. The study was carried out at the Biological and Chemical Research Centre, University of Warsaw, established within the project co-financed by European Union from the European Regional Development Fund under the Operational Programme Innovative Economy, 2007 - 2013.
LEACHING OF ARSENIC SPECIES IN INFUSIONS FROM HERBAL TEA COMMERCIALIZED IN BRAZIL

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Tea is one of the most consumed non-alcoholic beverages around the world. It is frequently associated to health benefits as prevention of heart diseases and low levels of cholesterol. Its nutritional composition is very rich and includes antioxidants compounds, several minerals and vitamins. However, inorganic contaminants may also found due to anthropic action in soil, wastewater and air. Arsenic is one of these contaminants and its speciation provides a decisive data: inorganic species (As III and As V) are known to be highly toxic while organic species, such as monomethylarsonic acid (MMA) and dimethylarsinic acid (DMA), present low toxicity. Considering this aspect, the aim of the present study was to establish a simple and fast method to analyze four arsenic species (As III, As V, DMA and MMA) in herbal leaves commercialized in Brazil and in their infusions as well as to evaluate the percentage of leaching of these species due to the infusion procedure. Eighteen samples of herbal tea (mix of flowers and fruits) were purchased from local markets in southeastern Brazil. Infusions were prepared using boiling water and the proportion of one sachet (1.5 g) to a cup (200 mL) was applied. Total arsenic were determined using microwave assisted digestion for herbal leaves and direct analysis using discrete sampling for herbal infusion by ICP-MS (power: 1.55 kW; isotope $^{75}\text{As}$, collision cell with 10 mL min$^{-1}$ of helium gas). Arsenic species were determined by HPLC-ICP-MS (anionic exchange column Hamilton PRP-X100, 4.1 x 250 mm, 10 µm; mobile phase: NH$_4$H$_2$PO$_4$ 20 mmol L$^{-1}$, 1.5 mL min$^{-1}$, pH 6.0 and injection volume: 100 µL) after sample preparation using microwave assisted extraction and dilution in mobile phase for herbal leaves and infusions, respectively. Total arsenic content in herbal leaves and infusions ranged between 30 and 1041 µg kg$^{-1}$ and <0.46 and 5.32 µg L$^{-1}$, respectively. Low extraction of arsenic from the herbal leaves to the infusions was verified considering that less than 20% (average) of the arsenic content was leached to the beverage. Inorganic species (As III and As V) were predominant representing 26 and 68% and 47 and 65% of total As content in herbal leaves and infusions, respectively.

Acknowledgements:
FAPESP (Process 2012/19142-7 and 2013/26855-2), CNPq, INCTAA and Agilent Technologies Brazil.
SAMPLE PREPARATION METHOD FOR MANGANESE SPECIATION IN *TRITICUM L.* BY HPLC-ICP MS

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Manganese is an element widespread in nature. Besides, it might be found as a different organic and inorganic species. The important role of manganese, as an activator of a several enzymes involved in photosynthesis, respiration and synthesis of proteins, acyl lipids and carbohydrates, in plants organisms is well known. Manganese can be accumulated in the leaf cell organelles, membrane fraction and roots, but an excess can lead to phytotoxicity \([1,2]\). The discovery of the relationship between the bioavailability and toxicity of manganese in plants becomes popular and makes manganese one of the target in speciation analysis, especially to understand mechanisms and to evaluate the impact of stress plants conditions and transport of manganese compounds \([3]\).

In speciation analysis, sample preparation plays essential role especially with respect to the problems with the stability of species and chosen analytical technique. The main aim of this work was focused on development of plant samples preparation for determination of manganese species using high performance liquid chromatography (HPLC) combined with inductively coupled mass spectrometry (ICP MS). Several extraction procedures for the isolation of water and protein Mn-fractions from *Triticum L.* (fresh, dry, freeze-dry and freeze samples) were tested. The efficiency of extraction was also assessed by determination of total manganese in plant by ICP-MS after microwave-assisted digestion of samples. The quality of used procedure was controlled by reference material of wheat – IPW 682 analysis. Ion pair and anion exchange chromatography were used to separate chosen manganese species in extracts prepared according to optimized procedure.

References
DETERMINATION OF ORGANIC AND INORGANIC SILICON SPECIES IN LIQUID ORGANIC SAMPLES USING WD XRF AND FAAS

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Determination of silicon in organic samples is a hot topic in atomic spectrometry [1-4]. Due to the element omnipresence there is a high risk of contamination of various materials, therefore the control of Si is necessary. Silicon is determined, among others in raw materials for catalytic processing of crude oil, in automotive fuels, bio-components and various solvents. Silicon can come from dust/soil (inorganic form, usually as SiO\textsubscript{2}) or from siloxanes/polydimethylsiloxanes (used as antifoaming agents). The effect of contamination can significantly depend on the Si chemical form. Generally, silicon dioxide, which is chemically inert, is expected to be less hazardous than Si in an organic form.

Lately [1], a methodological progress enabled to detect and determine about 100 various organic silicon compounds (Si content 0.1-40 mg kg\textsuperscript{-1}) in light petroleum products. However, if the sample is heterogenous and contains both organic and inorganic Si species, the present methodology offers only total amount of Si determination and the detection limit is at the level of 10 mg kg\textsuperscript{-1}.

In this work the Si determination in heterogenous samples was investigated. The samples were original petroleum products (for example: contaminated Diesel oil, used oils), bio-components coming from wastes processing as well as model samples prepared in laboratory. The analytical tools were wavelength-dispersive X-ray spectrometry and flame atomic absorption spectrometry. Various samples preparation procedures were evaluated, including mineralization and fusion. An analytical scheme of Si fractionation will be proposed.

References
HYDRIDE GENERATION WITH CRYOTRAPPING: DART-MS STUDY OF METHYLATED ARSANES AND ICP-MS ANALYSIS OF TRACE ARSENIC SPECIES IN WATER REFERENCE MATERIALS

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A technique of hydride generation (HG) with subsequent trapping of generated hydrides (cryotrapping, CT) under liquid nitrogen was developed in the early 1970’s to improve limits of detection for elements like arsenic and selenium. However, the unique features of this technique make it attractive even for modern analytical chemistry.

For studies of processes taking place e.g. in hydride generation or atomization, CT can effectively separate the species of interest from other compounds and also from accompanying ballast from HG- spray droplets, vapors and hydrogen. Presented examples are mass spectra of generated selenium hydride, arsane, mono-, di- and trimethylarsane from a DART ionization source coupled with an LTQ- Orbitrap mass spectrometer. Spectra in both positive and negative ion mode contain mainly the oxidized ions, with the hydride ion present as a minor ion if at all. Losses of one or more methyl groups are also observed for methyl substituted arsanes.

HG-CT offers the possibility of preconcentration of analyte from large sample volumes, as well as the ability to separate individual species. This is ideal for speciation analysis at ultratrace levels, which is one of the current challenges of elemental analytical chemistry. For many matrices, minimal sample pretreatment is required, which reduces sample dilution and risk of contamination.

The analysis of inorganic and methylated arsenic species is shown as an example of the sensitive detection achieved with HG-CT coupled to quadrupole ICP-MS. Results for new certified reference materials of river, sea and drinking water, with total arsenic content of 0.2- 1 µg L⁻¹, are presented.

Acknowledgement
This study was supported by Czech Science Foundation (P206/14-23532S) and the ASCR institutional support RVO: 68081715.
Chlorophylls have been analyzed for a long time. But still it is an uncertain field for reliable environmental analysis, especially in surface waters.

There is a correlation between the concentration of chlorophyll and the concentration of algae in water. The algae concentration depends on the water quality especially the (anthropogenic) nutrient concentration. The intervention of humans in the ecosystem surface water with nutrients from fertilizer leads to an enormous growth of algae which results in eutrophication of surface waters. By implication of knowing the concentration of chlorophyll we can describe indirectly the progress of eutrophication.

Chlorophylls can be found with a wide variety of structures and concentrations. Because of their structure, chlorophylls are active for UV/Vis-radiation. Therefore high performance liquid chromatography (HPLC) and further on thin layer chromatography (TLC) are used in the most separation experiments. The extraction of the chlorophylls is done according to common methods in environmental analysis of surface waters.

UV-VIS spectroscopy can detect different chlorophylls with a good sensitivity, but quantification is a problem because of the lack of reference substances and/or exact extinction coefficients for many chlorophyll species.

All chlorophylls contain a central magnesium ion, which can be detected by coupling of HPLC and flame atomic absorption spectroscopy (FAAS) and separated from non-magnesium-containing plant compounds. The objective of this study was to develop such a coupling method to separate various chlorophyll derivatives and to quantify them with high confidence. Therefore HPLC (Shimadzu LC prominence series) was coupled with FAAS (Shimadzu AA-7000).

In a second step, this quantification method by Mg ions was modified to a TLC-method. We succeeded in transferring the separated chlorophyll spots from TLC plates into GFAAS. Thus a cheap coupling from TLC-GFAAS was performed, enabling us to analyse and quantify Chlorophyll species even in ultratrases.

With the developed method the chlorophylls of different surface waters and leaf samples (stinging nettle, nori algae, red basil, purple beech) could be quantified. Although a senescence phenomenon was investigated.
APPLICATION OF SOLID PHASE EXTRACTION TECHNIQUE FOR MANGANESE SPECIATION ANALYSIS BY FLAME ATOMIC ABSORPTION SPECTROMETRY

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In this work, a new hyphenated technique developed from the coupling of solid phase extraction (SPE) and flame atomic absorption spectrometry (FAAS) for manganese ions determination is presented.

Recently, a lot of attention has been paid to SPE technique as a possible way to reduce matrix interferences via analyte transfer into a new media, as well as to achieve a preconcentration effect in order to get a significant increase of the analytical signal. Herein, this technique was applied for separation of cation and anion forms of manganese from water samples.

Manganese occurs naturally in surface and groundwater, yet in water management of manganese forms soil erosion process and anthropogenic sources play an important role. Mainly the following forms, labile Mn(II), particulate Mn(IV) and Mn(IV) hydroxide, can be found in the medium. The presence of manganese(VII) in water can be connected with the use of permanganate during water purification. Its higher concentration can cause e.g. disagreeable taste and stains at laundry.

We propose a SPE-FAAS technique for manganese speciation using two types of sorbents - activated silica gel and Dowex 1x4 which allow simultaneous retention and preconcentration of Mn²⁺ and MnO₄²⁻. A whole procedure is fully automated and realized in multicomutation flow system. Appropriate conditions like: type and concentration of eluent, or sample pH were found for both analytes. Proposed system allows determining manganese species in tap water samples with a good precision and accuracy.
SLURRY SAMPLING HYDRIDE GENERATION-CRYOTRAPPING-ATOMIC ABSORPTION SPECTROMETRY FOR ARSENIC SPECIATION ANALYSIS IN BABY FOOD

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The determination of trace and ultratrace element concentrations in commercially available baby foods is necessary to control the dairy intake of essential and potentially toxic elements. Among the toxic elements, arsenic takes a prominent place. Infants, toddlers and preschool children, consume relatively more food than an adult, when comparing the ratio of the mass ingested by body weight. Because of that, it is important to determine the arsenic content in baby food. The identity of arsenic species (inorganic and organic) controls their toxicity in food in general as well as in baby food. There are two inorganic arsenic forms, arsenite (iAs(III)) and arsenate (iAs(V)) and more than fifty organic arsenic compounds, among them the most abundant are methylarsonate (MAs), dimethylarsinate (DMAs) and trimethylarsine oxide (TMAso). While the methods for the determination of iAs(III) and iAs(V) are well-known, the determination of methylated species is not routine. An automated system for hydride generation-cryotrapping-atomic absorption spectrometry with multiatomizer (HG-CT-AAS), which was recently developed for arsenic speciation analysis in biological samples [1], has been applied for baby food slurry samples. In general, the use of HG AAS requires a sample pretreatment. Total sample dissolution is usually accomplished with the use of acids and microwave-assisted sample digestion in closed vessels. For arsenic speciation analysis, the use of strong oxidizing reagents such H\textsubscript{2}SO\textsubscript{4}, HClO\textsubscript{4}, HBr and/or aqua regia, besides being a time-consuming process, is not recommended in order to keep the integrity of the sample. In order to maintain the original speciation, the sample preparation using mild reagents has been evaluated. Slurry preparation procedures using HCl, HNO\textsubscript{3} and tetramethyl ammonium hydroxide (TMAH) with different concentrations were tested. The samples were placed in an ultrasonic bath for 15 min, heated at 85-90 °C for 20 min and placed again in the ultrasonic bath for more 15 min. The optimum conditions for sample preparation and arsines generation will be demonstrated.

Acknowledgements
CAPES, CNPq, Czech Science Foundation and Institute of Analytical Chemistry of the AS CR, v. v. i.

References
Here we report the results of a non-invasive population-based study that aimed to quantify Tl levels in 150 urine and 297 hair samples from the population of Valdicastello Carducci and Pietrasanta, Italy. In a recent study it has been shown the presence of thallium (Tl) at concentrations of concern in groundwater near Valdicastello Carducci (Italy). Tl contamination was also found in water intended for human consumption distributed in the same area, where it reaches 9 mg/L.

The present study aimed to i) quantify Tl with non-invasive sampling procedures; ii) correlate Tl levels found in hair and urine with Tl concentration in the tap waters used by inhabitants; iii) exploit the suitability of saliva as alternative matrix for environmental exposure studies. Quantification of Tl was performed by ICP-MS after pressurized microwave digestion, when necessary.

Thallium values found in urine and hair samples were correlated with Tl concentration levels found in tap water in the living area of each citizen and with his/her habits. Tl concentration is higher than 0.6 µg/L and 20 ng/g in about 50% of urine and hair samples, respectively. As Tl is generally removed from the body via urine, the high concentrations of Tl in the biological samples of the studied area must be ascribed to high accumulation of Tl through the food chain. The kinetics of decay of Tl concentration in urine samples was also investigated, finding that even 60 days after the end of the exposition, mean Tl urinary concentration was still extremely high.

Our findings indicate that people resident in the contaminated area significantly accumulated thallium in their urine and hair compared to the reference values of Italian population.
A COMPARISON OF THE RESULTS OF CHROMIUM DETERMINATION IN AUTOPSY TISSUES OBTAINED BY ET AAS AND ICP OES TECHNIQUES

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Elemental analysis of biological material serves a double purpose: determination of the concentration and profile of essential trace elements and detection of the presence of potentially toxic ones. In the routine toxicological studies on metal content, several analytical techniques can be applied, particularly flame and electrothermal atomic absorption spectrometry (FAAS and ET AAS, respectively), as well as inductively coupled plasma atomic emission spectrometry and mass spectrometry (ICP OES and ICP-MS).

On the base of a review of available literature on the determination of chromium in the different biological materials, it has been established that both the ET AAS and ICP OES techniques are commonly used for this analytical purpose, however, ET AAS has been recommended for reference concentrations of chromium [1].

In this study, a total of 70 samples, sections of internal organs (brain, stomach, liver, kidneys, heart and lungs) and blood, were tested for chromium using two of the above mentioned techniques. Prior to the analysis samples were wet digested in a microwave system using nitric acid and hydrogen peroxide. For the determination by ET AAS line 357.9 nm [1], and for ICP OES measurements emission lines: 267.7; 283.5; 284.3 and 357.8 nm were chosen (line 267.7 nm was recommended as analytical line for samples of biological origin by Nölte [2]).

It was found that the results obtained by the ICP OES were higher compared to those obtained by the ET AAS technique. However, statistically significant difference was demonstrated only for blood samples (concentrations determined using ICP OES were 20 times higher in this medium). Such differences in results obtained for blood samples may be caused by the presence of particularly high amounts of iron in this matrix, which can seriously interfere chromium signal during analyzes performed by ICP OES.

Based on performed analysis we concluded that the determination of chromium in biological samples at the levels of ng/g should be performed by ET AAS technique. ICP OES technique may only be used as a screening method to exclude the possibility of chromium poisoning.

References
CHEMICAL CHARACTERIZATION OF SHALLOW LAKES IN KAZAKHSTAN

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More than one third of Kazakhstan’s area is covered by lakes in the Central Asian region. Beside the well-known Aral Sea and Lake Tengiz there are several smaller permanent and intermittent shallow saline water bodies, which are very characteristic aquatic habitats. Despite the importance, there is a lack of knowledge in the field of chemical composition and ecology of these water bodies. The aim of our research was to measure specific electric conductivity and concentration of the eight major cations (calcium, magnesium, sodium, potassium) and anions (bicarbonate, carbonate, sulphate and chloride) in some Kazakh shallow lakes.

Temperature and depth were measured and samples were collected in 28 wetlands and saline lakes in North Kazakhstan. Specific electric conductivity was determined immediately after sampling applying a WTW Multiline P4 multimeter. The concentration of the eight major ions was measured in the laboratory. Calcium and magnesium were determined by atomic absorption spectroscopy, while concentration of sodium and potassium were measured by flame photometry. Bicarbonate and carbonate concentration was calculated from the results of alkalinity titration carried out both with phenolphthalein and methyl red–bromcresol green mixed indicators. Chloride was determined with argentometric titration. Sulfate was precipitated with barium chloride and measured spectrophotometrically. Based on the concentrations of the eight major ions equivalent percentages (e%) were calculated and ternary diagrams were prepared to compare the composition of the samples.

The specific electric conductivity values were between 1.3-235 mS/cm. It was found that in most of cases (in 25 cases out of the 28) sodium is the dominant cation in the investigated waters. In the case of three samples calcium was the dominant cation. (The concentration of the dominant cations varied in a wide range: it was 0.04-112 g/L and 0.08-5 g/L for sodium and calcium, respectively.) In 22 samples the equivalent percentage of chloride was the highest among the anions, the concentration of this ion varied between 0.06-195 g/L. In six other samples sulfate was dominant anion, the concentration of it was in the 0.17-27 g/L range. Based on the specific electric conductivity results most of the investigated water bodies were found to be hypersaline. Our results proved that the chemical composition of the investigated Kazakh saline lakes is different from the Hungarian soda pans, because the chloride and sulphate are dominant (more than 25 e% among the anions).
POSSIBILITIES TO INCREASE SENSITIVITY FOR FLAME AND FURNACE ATOMIC ABSORPTION SPECTROSCOPY USING AA-7000

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Nowadays, the aspect of “sensitivity” is accompanied by the elemental analysis, for example, the requirements for environmental protection or quality assurance are constantly increasing. Using the elements cesium and cadmium as example, there are various ways to improve the methodological parameters such as the detection and quantitation limit, which are highlighted within this poster.

For flame atomic absorption spectroscopy in addition to optimize gas flow rates, the atomic booster is applied. The atomic booster is a cylindrical quartz cell, which concentrates the analyte (atoms) within the optical pathway/light beam and increases the sensitivity by a factor of 2.5 to 5, depending on the element of interest.

Using graphite furnace atomic absorption spectroscopy, typically the furnace temperature program requires optimization steps, mainly depending on sample matrix. But there are several more options for method optimization available, like using the well-known omega platform tubes to increase sensitivity.

As last aspect the way how the graphite furnace is designed plays an important role for stable and sensitive measurements. With the GFA-7000A (Shimadzu), the digital controlled furnace enables higher long term stability due to intelligent temperature control and gas flow control; during atomization the atomic cloud remains a longer time in the optical pathway, increasing absorption values (Fig. 1).

Fig. 1: Intelligent gas flow control by GFA-7000A, Shimadzu
Wine is one of the oldest cultural products in human history. Wines have been cultivated for over 8000 years. The oldest known archaeological evidence of winemaking is an 8000-year old wine- and fruit press found near Damascus.

Winemaking is a rather simple process: freshly harvested grapes are crushed and the resulting juice (must) is collected. The must contains fermentable sugars and natural yeasts which, either by themselves or with the help of additional yeast cultures, start the fermentation process in which mainly ethyl alcohol and carbon dioxide are formed. The latter is a gas and escapes from the must. The fermentation process comes to a halt when all of the sugars are fermented or the alcohol concentration becomes too high and kills off the yeasts. At this point the must has turned into wine.

In order to guarantee a certain level of quality, standards are fixed in the national wine regulations such as the German “Weinverordnung” [1] from 21st April 2012, which includes the classification of wines from different locations but also the production process, alcohol concentrations and the maximum allowable concentrations of elements. A meticulous quality control procedure is essential, and during each stage of the production process analytical methods such as gas- or liquid chromatography, AAS-, ICP-, FTIR-, and UV-VIS spectroscopy as well as mass-spectrometry are applied for quality assurance or for product characterisation in order to guarantee the highest level of food quality as well as food safety.

Wine colour was measured at 520 nm using a UV-VIS spectrophotometer [2]. Quantitative determination of elements has been done with a Shimadzu ICPE-9820 ICP-OES spectrometer. Ultra fast analysis of resveratrol in red wine was done using the UHPLC- system with an RF-20Axs high-sensitivity fluorescence detector. The undesired 2,4,6-Trichloroanisole (TCA) in wine is detected using the headspace-trap GC/MS QP-2010 Ultra. Experimental data of a variety of methods will be presented.

References
As a result of environmental pollution and food chain, metals may be accumulated in human or animal bodies. Toxic metals cause inhibition on chemical and enzyme reactions in cells. Therefore, a negative situation forms in organs and tissues due to their toxic effects. The examination of metal pollution in foods and environment facilitates to monitor their harmful effects on human health. In the proposed study, the concentrations of toxic metals in tissue samples of animal obtained from a local farm were analyzed by inductively coupled plasma mass spectrometry (ICP-MS) following microwave-assisted digestion. Five different tissues - lung, liver, kidney, mussel and brain - were analyzed. Metals were differently distributed in the various organs, the highest concentration of Al was found in lung; Cu, Co and Mn in liver, Ni and As in kidney, V in lung and brain. Standard reference material (NIST SRM 2976 mussel tissue) was analyzed to check the accuracy of method.

Acknowledgement
This study has been supported by Cumhuriyet University Scientific Research Projects Commision as the research Project with the ECZ-005 code.
THE USE OF PLANTS OF THE GRAMINEAE FAMILY FOR THE REMEDIATION OF ASH LANDFILL

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Production of electricity in Poland is based mainly on coal. As a result there are gained large amount of bottom ash. There are several methods to apply bottom ash in other branches of industry. It is used in ceramic industry, concrete production, mining or agriculture and others. Unfortunately in most cases bottom ash is store in landfills [1].

Because of its nature it may have had adverse results on environment. Heavy metals are capable to condensation on the ash particles during combustion of coal. Furthermore, PAH compounds are adsorbed on the surface of the particles. Rainfall leaches these compounds and causes their migration to soil and groundwater. Other problem is volatility of bottom ash what forces to applying additional protection actions [2].

One of the opportunities is phytoremediation. In our research was applied one of the Gramineae family plant – Triticum (spring wheat of the Tybalt variety). The aim of this work was to verify accumulation ability of selected elements (cadmium, calcium, cupper, iron, manganese, nickel, zinc) in above-ground parts of the plant and in its roots alike. For this purpose, there were prepared pot cultures experiments on pure soil, pure bottom ash and 5 kind of ash-soil mixtures: 95%-5%; 90%-10%, 80%-20%, 70%-30%, 50%-50%, bottom ash-soil (m/m), respectively. To each pots was added 30 seed of the wheat. The plants were growing through 3 weeks. Then, they were drawn from the ground and washed up in tap water and in deionized water. The next step was separating roots and above-ground parts each other and left to dry in the air. After preliminary drying, plants were cut into pieces and transferred into weighing bottles. Then they were dried at 70°C to constant mass. Such prepared samples were digested in the mixture of nitric acid and hydrochloric acid (6 ml:1 ml, respectively). The digested mixture were carried on to a volumetric flask and filled to mark. Then the digests were filtered to plastic container. Determination of total content of previously mentioned elements were performed with Flame Atomic Absorption Spectroscopy (Ca, Cu, Fe, Mn, Zn) and Electrothermal Atomic Absorption Spectroscopy. It was found that metals under study were accumulated mainly in roots of wheat. A significant correlation between content of metal in roots and stems has been observed for Cu and Zn. The addition of alkaline bottom ash to the soil causes a decrease in copper and zinc bioavailability.

References
The rare earth elements have become emerging contaminants in marine and terrestrial environment. As they are the high-technology metals applied in many modern devices and advanced industrial processes they have been released from the ores to the other “mobile” components of environment having a potential effect on human health.

Because of their low natural background concentration and their unique element signature (a profile showing the contents of the lanthanides), anthropogenic input can be followed through the waste water discharge into the rivers, the coastal waters and open oceans thereafter.

Despite the fact of the great technological progresses in development of analytical methods over the past years, quantifying REEs in many environment samples still remains a challenging task. The major problems to overcome during quantitative determination of REEs are their low or ultra-low concentrations, complex matrices and sample preparation procedures.

The inductively coupled plasma mass spectrometry technique (ICP-MS) allows performing multielemental, fast and ultra-low level determination of REEs concentrations in different samples. However, due to their low content and the high concentration of interfering matrix components determination of REEs in the environmental samples requires very often pre-concentration and separation step (e.g. analysis of seawater).

In the present study two analytical procedures for the analyses of REEs in natural seawater samples has been developed and compared. The off-line seaFAST pre-concentration device and the on-line APEX introduction system combined with high resolution sector field inductively coupled plasma mass spectrometry (ICP-SFMS) were used for determination of REEs in environmental water samples.

The method validation was effectuated according to the requirements of ISO-17025 standard. Thereupon, procedural blanks, selectivity, calibration curve, linearity, working range, recovery, precision, traceability and limits of detection and quantification were assessed for both proposed methods. The estimation of the total uncertainty associated to each measurement result was fundamental tool for sorting the main sources of measurement biases. All major sources of uncertainty were identified and propagated together following the ISO/GUM guidelines. The uncertainty contributions and the results obtained with these two analytical procedures were compared and evaluated for their intended application.
Macro- and micro elements in wines are present in form of metal ions that take part in the composition of the thousands of various molecules available in wines. Metal ions are present in „natural form” – mostly bound to acids, thus they can be easily enter into the human metabolism pathway. Thus, moderate consumption of wine provides a „nicely packaged multivitamin product” – a source of minerals and trace elements for us.

Effect of yield regulation on the components of wine has been examined by our research team for years. Measurement of pH plays a very important role in acid composition and acid harmony, but also in yield regulation. Information in literature related to the examination of the latter one is scarce.

Effects of yield regulation in 2013 vintage on poliphenol elements and also on some inorganic macro- and micro elements were examined by AAS. According to our results, Ca\(^{2+}\) and K\(^{+}\) ion content were correlated with organic acid and poliphenol content of wines.

- It can be stated that in the case of higher acid content and lower pH, Ca\(^{2+}\) and K\(^{+}\) ions show lower concentration, while in the case of higher mineral content, pH value also increases. This has been proven also in our experiments from yield regulated Kékfrankos and Merlot grapes.

- No significant increase or decrease has been detected in the changes of pH and total acid content in relation to total poliphenol, anthocianin and leukoanthocianin values.

- Our yield regulation experiments have proven that an optimal value must be set in yield regulation and environmental conditions (terroir), but also right timing of harvest and wine-making technology are essential.
Atomic mass spectrometry with ionization by inductively coupled plasma and laser ablation sampling (LA-ICP-MS) is widely applied for direct analyses of solid materials, yet in order to obtain quantitative results, it requires an accurate, frequently complex, calibration approach [1]. Since one of the most promising features of LA-ICP-MS is the possibility of almost direct analysis of different solid samples, with significantly limited step of sample preparation, it is highly desirable to make the calibration as simple as feasible. Nevertheless, in this case accurate determinations can be complicated due to matrix effects, fractionation and little sample throughput, which leads to analytical signals of low intensities and stability.

Application of this technique towards analysis of distribution of selected elements in bones is a challenging task mainly due to strong morphological diversification, incident to bones diagenesis. However better understanding of ablation process and interpretative possibilities in the area of anthropological studies are the main reasons weighted in favour of taking a try to determine concentration of selected elements in this material.

In order to examine whether the matrix – matching is indeed crucial for obtaining accurate and precise results, different procedures of standards preparation were developed and applied. In the first approach, matrix – matching was accomplished by use of real bone material, milled and spiked with SRM 987 (strontium carbonate). In this case, so called combine standard addition method was applied for calibration. The method incorporates two approaches – extrapolation (standard addition) and conventional interpolation (set of standards). Next, to simulate the matrix, standards were prepared with a use of hydroxyapatite (HA), again spiked with SRM 987. The second procedure allowed preparing a blank sample. Those two procedures were confronted with a non matrix – match approach, where thin layers of strontium standard solutions were deposited on the microscopic glasses and dried in a room temperature.

The quality of prepared standards was checked in terms of analytical signals stability and accuracy, while comparing with the average concentrations obtained through the pneumatic nebulization PN-ICP-MS analysis of the standards digested in a nitric acid with an assistance of microwave radiation.

Finally, prepared standards were applied to calibration of solid bones analysis by LA-ICP-MS. Analytical signals were mathematically corrected with regard to the interferential influence of $^{87}\text{Rb}$ on $^{87}\text{Sr}$. Obtained results were compared and evaluated in terms of accuracy.

References
ETV-ICP-OES: A POWERFUL TOOL FOR DIRECT MULTIELEMENTAL ANALYSIS OF LITTLE AMOUNTS OF BIOLOGICAL SAMPLES

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In the case of biologically samples analyses for environmental, forensic, biomedical and/or clinical and other applications the common difficulty is the very small amount of material available for sampling. The connection of fully simultaneous ICP-OES (inductively coupled plasma - optical emission spectroscopic) system capable of rapid transient signal processing with sophisticated ETV(electrothermal vaporization)-device allows the rapid direct analysis including major, minor and trace elements from low sample amount (a few milligrams or less depending on properties of matter) without any mineralization and/or other treatment steps. Only the drying step was used in the case of wet samples. The technique allows the combined, matrix-matched or matrix-free calibration with home-made or certified solid and aqueous standards. For example, the ETV-ICP-OES technique was used in IOCB analytical service-laboratory in the following studies:

1/ Only boron or together boron and cobalt contents were directly estimated in fresh frozen mice tissues for tracking the carboran-based candidate-drugs and for their pharmacokinetic evaluation.

2/ The amounts of heavy metals and other elements in the collected insect samples from both polluted postindustrial and healthy areas were determined. Based on the use of atypically, less sensitive lines, the simultaneous analysis of macro- and trace-elements is possible. 44 separated analytical lines for totally 18 elements (Ag, Al, As, Ba, Ca, Cd, Co, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Še, Sr, V a Zn) were simultaneously monitored, calibrated and used for measurement of about 1 mg dried and grounded insect sample aliquots.

3/ A method for determination of biologically important major (Ca, K, Mg, P) and minor elements (Ba, Co, Cu, Fe, Mn, Na, Sr, Zn) in plants was developed.

The LODs’ in all developed applications ranged from 0,001 mg/kg for trace metals (e.g. Co) to 490 mg/kg for K in dry plant material (measured concentration values in % range). The typical RSD values were less than 10 % depending on material homogeneity and the recovery-range by certified material analysis was in the range 89 – 112 %.
DETERMINATION OF ANTIMONY USING ELECTROCHEMICAL HYDRIDE GENERATION IN COMBINATION WITH HRCS-AAS

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Antimony occurs naturally in the environment. In unpolluted waters typical concentrations of dissolved antimony are less than 1 μg l⁻¹. However, in the proximity of anthropogenic sources, concentrations can reach up to 100 times of natural levels. Antimony occurs naturally in environmental samples in two oxidation states as Sb(III) and Sb(V) in inorganic and organic components. Speciation of antimony is important for environmental studies for its biological behavior and toxicity depend on its oxidation state. Generally, inorganic antimony is more toxic than organic antimony and Sb(III) is 10 times more toxic than Sb(V) species.

The paper is focused on the determination of antimony in aqueous solutions using electrochemical preconcentration and hydride generation and determination by high resolution continuum source atomic absorption spectrometry (HRCS-AAS). The electrochemical hydride generation involved two principal steps. The first step was the deposition of antimony in a porous glassy carbon cathode as elemental antimony. In the second step, antimony was converted to stibine at the same electrode surface, then was transported by argon gas to the quartz cuvette of the spectrometer. This approach does not require any chemical reductant just acids of high purity, thereby greatly reducing the risk of contamination by reagents and the cost of analyses.

The effects of several parameters on electrochemical hydride generation system were investigated such as the cathode material, anolyte and catholyte solutions, carrier gas flow rate, applied current. The analytical figures of merit, accuracy of the technique and its resistance to some transition and hydride forming elements were evaluated. The detection limit and accuracy of the method are below 1 μg l⁻¹ and 3.5 %, respectively. Analysis of various water samples was carried out to demonstrate the performance of the method.

Acknowledgments
The financial support by the Competence Center for SMART Technologies for Electronics and Informatics Systems and Services, ITMS 26240220072, and the grant agency VEGA (project No. 1/0491/16) is highly appreciated.
MULTI-ELEMENT ANALYSIS OF ACID MINE DRAINAGES BY USING INDUCTIVELY COUPLED PLASMA–MASS SPECTROMETRY WITH COLLISION-REACTION CELL TECHNOLOGY

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Collision-reaction cells are accepted as the preferred means for removing of spectral interferences in quadrupole ICP-MS. They can promote reactive and non-reactive collisions, with resultant benefits in separation of the sample matrix and reduction of isobaric and polyatomic interferences. This chemical resolution technique can avert interferences, requiring the use of the high resolution mass spectrometer.

In this work, the analytical technique ICP-MS equipped with an octopole collision-reaction cell (ORC) for the multi-element analysis of acid mine drainages from the old mining works of Slovakia was used.

The technologically and environmentally interesting elements of studied sample matrix were determined (Mg, Al, Mn, Fe, Co, Cu, Zn, As, Sr, Cd and Pb), and the basic validation characteristics were estimated. Analyses were performed in optimal experimental conditions for ICP-ORC-MS. Accuracy of the method was verified by the certified multi-element standard. Variability of recoveries of the control sample was evaluated (from 96 to 105%). Accuracy was further estimated by comparison of the results of element analyses for real samples, obtained by the next independent method (AAS). The variability of recoveries, with regard to the reference method, ranged from 95 to 107%. Precision (as repeatability) was evaluated, and RSDs were ranged from 1 to 8%. Limits of detection (3σ-criterion) varied for the studied elements in the range from 0.001 to 0.119 µg l⁻¹. In accordance with the requirements for analysis, the optimal calibration range was chosen (up to 100 µg g⁻¹ for all studied elements).

Keywords: Octopole Collision-reaction Cell, ICP-MS, Inorganic Mass Spectrometry, Environmental Analysis, Acid Mine Water

Acknowledgements:
The work was created with the financial support of the Operational Programme Research and Development - Project: Centre of excellence for integrated research into the Earth’s geosphere (ITMS: 26220120064), which is co-financed by the European Regional Development Fund.
DERIVATIVE SPECTROSCOPIC DETERMINATION OF
FLORFENICOL IN SOME NATURAL SAMPLES

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Florfenicol, 2,2-dichloro-N-((1R,2S)-3-fluoro-1-hydroxy-1-(4-(methylsulfonyl)phenyl)propan-2-yl)acetamide has the chemical structure:

Florfenicol is a member of chloramphenicol and thiamphenicol family. The chemical name is 2,2-dichloro-N-[(1R,2S)-3-fluoro-1-hydroxy-1-(4-methanesulfonyl)phenyl]propan-2-yl] acetamide. Florfenicol was widely used clinically now for the treatment of intestinal infections, respiratory tract infections, typhoid, and so on. Compared to thiamphenicol, florfenicol shows significant superiority in antibacterial spectrum, antibacterial activity, and considerably lower side effect; its antibacterial potency is 10 times higher than that of thiamphenicol. A new, simple, rapid, wide applicable range and reliable derivative spectrophotometric method has been developed for determination of enrofloxacin.
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