



CECE 2013

10TH INTERNATIONAL INTERDISCIPLINARY
MEETING ON BIOANALYSIS



PROGRAM AND ABSTRACTS

APRIL 25-27, 2013

PÉCS

HUNGARY



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PROGRAM and ABSTRACT BOOK

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Welcome to this year's CECE

This symposium is the tenth in the series of the traditional symposia organized previously in Brno, Czech Republik, starting with only a few lectures at the Institute of Analytical Chemistry in 2004.

This year the symposium is honoured by the opportunity to celebrate Professor Stellan Hjertén for his 85th birthday.

The symposium visits, the third time, Pécs, which was the Cultural Capital of Europe in 2010.

Since its start it was the aim to create an interdisciplinary meeting for informal communication of scientists from different sides of bioanalytical sciences. The Symposium is now a serious member of the meetings of scientists, since it is continuously growing in research areas and number of participants, which gives great opportunity for discussions and presentations of new results in bioanalytical science.

It is expected that this conference will further contribute to the exchange of ideas and will provide a forum for stimulating discussions.

The organizers want to thank you for your participation and hope that you will enjoy the scientific presentations, personal contacts and informal discussions.

<http://cece2013.pte.hu>

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Rector's greeting

It is my pleasure to welcome you at the University of Pécs!

The University of Pécs is one of the largest institutions of higher education in Hungary with the widest spectrum of teaching and research activities that is known and recognised even beyond our borders. Our University represents and accepts as its own a long tradition dating back to the Middle Ages, while at the same time it also plays an active role in the task of institutionalising new knowledge that is aimed both for the present and the future.

With our more than 500 different study programmes our main goal is to ensure high-level teaching and research activity in every possible area of study, assist the 27,000 students studying here as much as possible during their student life, organize study abroad scholarships and maintain and improve the quality of the university services.

The academic year of 2012/2013 has special significance in the history of the University of Pécs, as we not only celebrate the centennial of the foundation of the Hungarian Royal Elizabeth University of Pozsony, but also the 90th anniversary of its move to Pécs. Our success and results so far speak for themselves and require increased efforts and continuous renewal from us.

The aim of this conference - bringing together experts from different disciplines, to discuss recent progress in this particular field and stimulate collaborative efforts - is also one of the most important objectives of the University of Pécs. The mission of the University of Pécs as a regional knowledge base is to develop innovation-oriented and knowledge-based economy, create the environment that is necessary for the optimal flow of knowledge.

It is an exceptional pleasure to greet our *Honoris causa doctor*, Professor Wilhelm Einar Stellan Hjertén, at this conference, who have had – in several form – a long and fruitful collaboration with University of Pécs. His support and encouragement helped several of his past and recent co-workers, also from our University, to receive high-ranking international reputation.

I do hope that you will find the conference useful in learning more about development and application of bioanalysis and you can obtain specific knowledge that will play a determinant role in your future professional life:

Prof. Dr. József Bódis

Rector of the University of Pécs

Organizing Committee

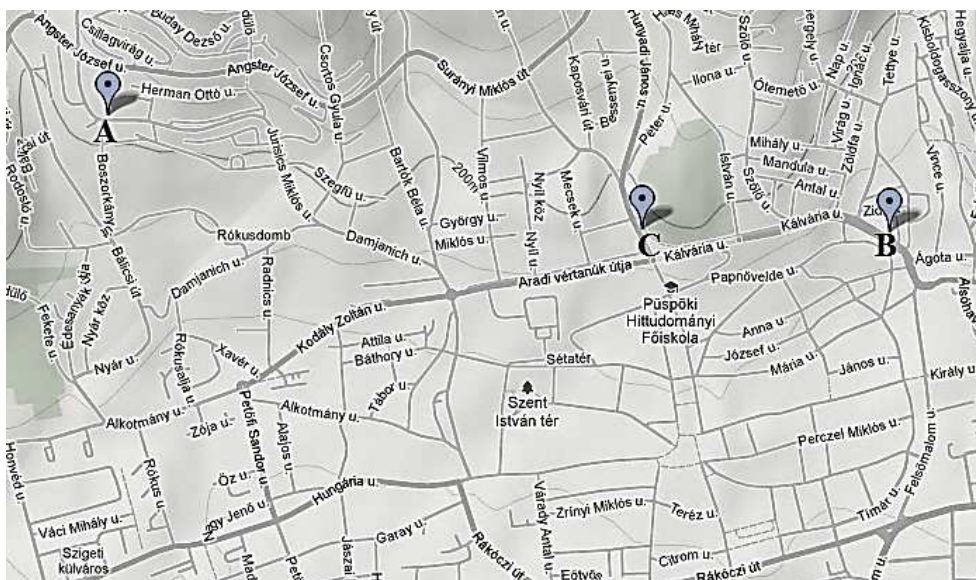
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Laura Nagy
Ildikó Merk
Ibolya Kiss
Balázs Csóka

Regional Center of the Hungarian Academy of Sciences

University of Pécs, Institute of Bioanalysis
and
Department of Analytical and Environmental Chemistry

Venue

The symposium will held at the
Regional Center of the Hungarian Academy of Sciences
7624 Pécs, Jurisics Miklós Street 44.



- A:** The location of the conference: Regional Center of the Hungarian Academy of Sciences
- B:** Kálvária-Rác Hotel
- C:** Bus stop: You can go from here with the bus number 32, and you have to travel to the "MTA székház" station (5th station from here).

Accommodation

The participants are accommodated at the Kálvária-Rác Hotel (7625 Pécs, Kálvária u. 6.) and at the Regional Center of the Hungarian Academy of Sciences (7624 Pécs, Jurisics Miklós út 44).

Program schedule

April 24, 2013 - Wednesday		Arrival
April 25, 2013 - Thursday	14:00	Doctoral forum for young researchers
April 26, 2013 - Friday	8:30	Opening Ceremony
	9:00	Lectures
	12:50	Lunch
	14:00	Poster-discussion
	15:00	Lectures
	18:00	Trip to Villánykövesd - Symposium dinner
April 27, 2013 - Saturday	9:00	Lectures
	14:20	Closing the symposium
	14:30	Lunch
	15:30	Sightseeing - Pécs
April 28, 2013		Departure

Opening hours of the registration desk

April 25, 2013: 12:00-16:00

April 26, 2013: 8:00-12:00

Social program

The symposium dinner will take place in **Blum Pince** at Villánykövesd on Friday.

On Saturday after the lectures you can participate in a Guided Tour in Pécs.

April 25, Thursday

Forum of Doctoral School of Chemistry

- 14:00–14:15 *Nándor Lambert*, Attila Felinger*
DF-01 **Comparison of overall mass-transfer coefficients of Supercritical Fluid Chromatography and Liquid Chromatography**
- 14:15–14:20 Discussion
- 14:20–14:35 *Csaba Szmolnik*, Wolfgang Lindner, Attila Felinger*
DF-02 **Investigation of the retention phenomena of Mefloquine enantiomers: effect of the eluent composition**
- 14:35–14:40 Discussion
- 14:40–14:55 *Annamária Sepsey*, Ivett Bacskay, Attila Felinger*
DF-03 **Modeling Wide Pore size distributions in Size Exclusion Chromatography**
- 14:55–15:00 Discussion
- 15:00–15:15 *Anikó Kőnig-Péter*, Tímea Pernyeszi*
DF-04 **Comparison of biosorption processes by bacterial and alga cells**
- 15:15–15:20 Discussion
- 15:20–15:35 *László Kiss, Zsuzsanna Óri*, Lívía Nagy, Géza Nagy*
DF-05 **Modified, layer coated amperometric sensor for measuring in natural, porous matrices**
- 15:35–15:40 Discussion
- 15:40–15:55 **Coffee break**
- 15:55–16:10 *Péter Szabó*, János Kovács, László Kocsis*
DF-06 **Preliminary results for the stable isotope composition of Late Pliocene environment in fossil *Stephanorhinus* sp. and *Mammut* sp.**
- 16:10–16:15 Discussion

- 16:15–16:30
DF-07 *Paweł Pomastowski*, M. Sprynskyy, M. Gawin, W. Piekoszewski, B. Buszewski*
A study of zinc-binding to casein in lights of potential medical application
- 16:30–16:35
Discussion
- 16:35–16:50
DF-08 *Li Xu*, György Csekő, Tamás Kégl, Attila K. Horváth*
Kinetics and mechanism of the pentathionate-iodine reaction
- 16:50–16:55
Discussion
- 16:55–17:10
DF-09 *Viktor Sándor*, Dalma Scheffer, Ferenc Kilar, Béla Kocsis, Ágnes Dörnyei, Anikó Kilar*
Electrophoretic and mass spectrometric analysis of bacterial endotoxins
- 17:10–17:15
Discussion

April 26, Friday

- 8:30-9:00 **Opening Ceremony**
Greetings to Professor Stellan Hjertén
- Session I** *Chairman: Ferenc Kilár*
9:00-9:25 *Stellan Hjertén*, Liao, J. L., Wang, Y.*
L-01 Uppsala University, Uppsala, Sweden
The artificial counterpart of the native protein antibody
9:25-9:35 Discussion
- 9:35-10:00 *Johan Roeraade*, Patrik Ek and Johan Jacksén*
L-02 KTH - Royal Institute of Technology, Stockholm, Sweden
Ideas, trials and progress in the analysis of low-abundant biomolecules
10:00-10:10 Discussion
- 10:10 **Coffee Break**
- Session II** *Chairman: Ákos Végvári*
10:30-10:55 *Gabriel Peltre*, H. Senechal, P. Poncet*
L-03 Hopital Trousseau, Biochemistry Lab, Paris France
Diversity of allergens and of the antibodies raised to them, a challenge for bioanalytical methods
10:55-11:05 Discussion
- 11:05-11:30 *František Foret*, Petra Jusková, Pavel Podešva*
L-04 Institute of Analytical Chemistry, AS CR, Brno, Czech Republic
Thin metal layers in bioanalysis
11:30-11:40 Discussion
- 11:40-12:05 *C. Ibáñez, A. Valdés, V. García-Cañas, C. Simó, Alejandro Cifuentes**
L-05 Laboratory of Foodomics, CIAL (CSIC), Madrid, Spain
A metabolomic study of the antiproliferative effect of carnosic acid against human colon cancer cells
12:05-12:15 Discussion
- 12:15-12:40 *Ferenc Kilár*, Anikó Kilár, Viktor Sándor, Lilla Makszin, Ágnes Dörnyei, Béla Kocsis*
L-06 University of Pécs, Pécs, Hungary
Lipopolysaccharidomics – A complex approach
12:40-12:50 Discussion

12:50	Lunch
14:00–15:00	Poster discussion <i>The authors are requested to be present at their posters during the Poster discussion.</i>
Session III	Chairman: Stellan Hjertén
15:00–15:25	<i>Ákos Végvári*</i>
L-07	Clinical Protein Science & Imaging, Dept. of Measurement Technology and Industrial Electrical Engineering, Lund University, Lund, Sweden
15:25–15:35	Drug localization in tissue sections by MALDI-MS imaging Discussion
15:35–16:00	<i>Melinda Rezeli*</i>
L-08	Clinical Protein Science & Imaging, Lund University, Lund, Sweden
16:00–16:10	Quantitative proteomics applied to biobanking material Discussion
16:10–16:35	<i>Mantas Stankevičius, Ieva Akuneca, Tomas Drevinskas, Vilma Kaškonienė, Rūta Mickienė, Kristina Bimbraitė-Survilienė, Gražina Juodeikienė, Dalia Cizeikienė, Elena Bartkienė, Ona Ragažinskienė, Audrius Maruška*</i>
L-09	Department of biochemistry and biotechnologies, Vytautas Magnus University, Kaunas, Lithuania
16:35–16:45	Increased biological value and safer food product development using solid state fermentation of plant material with bacteriocins-producing lactic acid bacteria: comparative phytochemical analysis of fermented and non-fermented samples Discussion
16:45–17:10	<i>Kjell-Ove Eriksson*, E. Heldin, E. Hallgren, J. Shanagar, S. Grönlund, H. Tunes, M. Xavier, L. Vilela</i>
L-10	GE Healthcare Bio-Sciences AB, Uppsala, Sweden
17:10–17:20	Development of intermediate purification step in insulin process using a high throughput approach Discussion
18:00	Trip to Villánykövesd - Symposium Dinner

April 27, Saturday

- Session IV**
9:00–9:25
L-11
- Chairman:* Attila Felinger
*Karel Kleparnik**
Institute of Analytical Chemistry - Academy of Sciences of
Czech Republic, Brno, Czech Republic
- Single cell analysis: State of the art**
Discussion
- 9:25–9:35
- 9:35–10:00
L-12
- Marianthi Kafentzi, Yasmina Mekmouche, Eloïne Npetgat,
Viviane Robert, Pierre Rousselot Pailley, Ludovic Schneider,
Jalila Simaan, Thierry Tron**
Aix-Marseille Université, Marseille, France
- Engineering laccases: in search for new biocatalysts**
Discussion
- 10:00–10:10
- 11:10–11:35
L-13
- Róbert Berkecz, Zoltán Szabó, Zoltán Kele, Tamás Janáky**
University of Szeged, Szeged, Hungary
- Identification peptides against Alzheimer's disease: a
proteomic approach**
Discussion
- 10:35–10:45
- 10:45–11:05
L-14
- Szőkefalvi-Nagy*, Zoltán, I. Kovács*
Institute for Particle and Nuclear Physics, MTA Wigner
Research Centre for Physics, Budapest, Hungary
- Elemental analysis of protein by ion beam bombardment**
Discussion
- 11:05–11:15
- 11:15–11:30
Coffee Break
- Session V**
11:30–11:55
L-15
- Chairman:* František Foret
*Attila Felinger**
Department of Analytical and Environmental Chemistry,
University of Pécs, Pécs, Hungary
- Molecular approaches for the investigation of mass transfer
phenomena in chromatography**
Discussion
- 11:55–12:05

- 12:05–12:30
L-16 *Alberto Cavazzini**, *Nicola Marchetti*, *Luisa Pasti*, *Francesco Gasparrini*
University of Ferrara, Department of Chemistry and
Pharmaceutical Sciences, Ferrara, Italy
**New insights into the retention mechanisms on straight-
chain perfluorinated stationary phase for HPLC**
- 12:30–12:40 Discussion
- 12:40–13:05
L-17 *Andrea Nagy*, *Attila Gáspár**
Department of Inorganic and Analytical Chemistry, University
of Debrecen, Debrecen, Hungary
**Designing and preparation of multiple chromatographic
packings in microchip**
- 13:05–13:15 Discussion
- 13:15–13:40
L-18 *Ana Fernandez-la-Villa**, *Vanesa Bertrand-Serrador*, *Diego F. Pozo-Ayuso*, *Mario Castaño-Alvarez*
Severo Ochoa Building, Asturias, Spain
**Fast and reliable urine analysis using a portable platform
based on microfluidic electrophoresis chip with
electrochemical detection**
- 13:40–13:50 Discussion
- 13:50–14:10
L-19 *Alexander Jönsson*, *Loreta Bllaci*, *Sven Kjellström*, *Sandra Lemos*, *Lena Eliasson*, *James R. Friend*, *Leslie Y. Yeo*, *Staffan Nilsson**
Pure & Applied Biochemistry LTH, Lund University, Sweden
Open chip SAW-MALDI MS sample handling
- 14:10–14:20 Discussion
- 14:20 **Closing the Symposium**
- 14:30 **Lunch**
- 15:30 **Guided Tour in Pécs**

Posters

- P-01** *Ivett Bacskay*, Annamária Sepsey, Attila Felinger*
Experimental validation of the molecular theory of size-exclusion chromatography with wide pore size distribution
- P-02** *Endre Bartó*, Ibolya Prauda, Ferenc Kilár, Attila Felinger, Ibolya Kiss*
Application of cavitand derivatives on high performance liquid chromatography
- P-03** *Andrea Nagy*, Attila Gáspár*
Fabrication of microchips with multichannel systems
- P-04** *Melinda András*, Brigitta Törzsök, Álmos Klekner, Attila Gáspár*
Determination of temozolomide in serum and brain tumor with micellar electrokinetic capillary chromatography
- P-05** *V. Juhász, E. Beéry, Z. Nagy, A. Bui, É. Molnár*, A. Csorba, Z. Timár, J.K. Zolnerciks, R. Magnan, Sz. Czvik, M. Jani, P. Krajcsi*
Determination of the OAT1, OAT3 and BCRP substrate chlorothiazide by LC-MS/MS
- P-06** *Éva Pósfai*, Imelda Marton, Balázs Kotosz, Márta Széll, Zsuzsanna László, Zita Borbényi*
Identification of MPL-W515L mutation in thrombopoietin receptor - could be „MPL-W515L mutation an additional vascular risk factor” in woman diagnosed with essential thrombocythemia
- P-07** *Viktor Farkas*, Ferenc Kilár, Borbála Boros, Attila Felinger, Tímea Pernyeszi*
Influence of culture parameters on phenol biosorption by lyophilized mycelial pellets of phanerochaete chrysosporium
- P-08** *Lívía Nagy, Daniel Filotás*, Melinda Boros, Erika Pintér, Géza Nagy*
Development and investigation of subcutaneous hydrogen sulfide (H₂S) absorption using micro biosensor

- P-09** *Krisztina Honfi*, Ferenc Kilár, Tímea Pernyeszi*
Biodegradation and adsorption properties of candida tropicalis cells in aqueous solutions
- P-10** *István Ilisz*, Dénes Zádori, Péter Klivényi, István Szatmári, Ferenc Fülöp, József Toldi, László Vécsei, Antal Péter*
Development and application of LCMS and LC-FLD methods for the analysis of kynurenic acid and a novel kynurenic acid analog in mouse serum
- P-11** *Tamás Jakó*, Zsolt Wagner, Tamás Tábi, Gergely Zachar, András Csillag, Éva Szökő*
Analyzing glutamate and aspartate enantiomers in brain tissue samples by CE-LIF
- P-12** *Zoltán Kele*, Györgyi Váradi, Gábor Tóth*
Strategy for identification of disulfide bridges in a cysteine rich protein
- P-13** *Tamás Kiss*, Lilla Makszin, Ágnes Blaskó, Victor U. Weiss, Ferenc Kilár*
Zone electrophoresis on microchip for biomolecules
- P-14** *Ibolya Kiss*, Nándor Lambert, Ferenc Kilár, Attila Felinger*
Retention and mass-transfer properties of insulin on superficially porous and totally porous reversed phases in HPLC
- P-15** *M. Stankevičius*, A. Maruška, T. Drevinskas, M. Kazlauskas, N.Tiso, J.Mikašauskaitė, I.Akuneca, V.Bartkuvienė, O.Kornyšova, K.Barčauskaitė, V.Snieškienė, A.Stankevičienė, O.Ragažinskienė, D.Levišauskas*
Screening of used wooden railway sleepers chemical composition by means of gas chromatography – mass spectrometry
- P-16** *Krisztina Németh*, Celesztina Nagy-Domonkos, Jayapal Reddy Mallareddy, Virág Sarnyaia, Géza Tóth, Julianna Szemán, László Jicsinszky, Lajos Szenté, Antal Péter and Júlia Visy*
Stereoselective analysis of amino acids and endomorphin analogue tetrapeptides by capillary electrophoresis

- P-17** *Paweł Pomastowski*, B. Buszewski, K. Hrynkiewicz, M. Gawin, W. Piekoszewski*
Determination of selected bacterial proteins from 2-D SDS-PAGE by using MALDI-TOF-MS
- P-18** *Emőke Szerdahelyi*, András Nagy, Eszter Korompai, Éva Gelencsér*
Determination of meat originated imidazole dipeptides by CZE
- P-19** *Tea Perkov*, Jasmina Rokov Plavec, Lilla Makszin, Ferenc Kilár*
Microchip capillary electrophoresis in expression profiling of circulating tumor cells from cancer patients
- P-20** *Ieva Akuneca, Mantas Stankevičius, Tomas Drevinskas*, Audrius Maruška, Ona Ragažinskienė, Vitalis Briedis, Kristina Ramanauskienė, Ada Stelmakienė, Rasa Ugenskienė*
Phytochemical analysis and classification according to growth sites in Lithuania of *Chamerion angustifolium* L. Using chromatographic and related techniques
- P-21** *Zoltán Pápai, Ágnes Bóna, Gábor Maász, János Schmidt, Éva Jámbor, Róbert Ohmacht, László Márk**
Investigation of trans-resveratrol and stilbene derivative TDPA in hungarian wines using HPLC-MS
- P-22** *Zoltán Pápai*
LC-MS analysis of dopamine metabolites in brain
- P-23** *Pavel Podesva; Frantisek Foret*
Thin metal films in resistivity-based chemical sensing

Invited speakers



Alberto Cavazzini, born in Ferrara (Italy), received his PhD (2000) from the University of Ferrara (Ferrara, Italy). He spent two years at the University of Tennessee in Knoxville (Knoxville, TN, USA) as post-doctoral fellow in the group of professor G. Guiochon. Since 2001, he holds the position of research associate at the University of Ferrara. Main research interests are in the field of linear and nonlinear high performance liquid chromatography (HPLC) for: (1) separation/purification of optically active molecules, biomolecules, etc.; (2) characterization of new stationary phases and adsorption media; (3) modeling of liquid-solid and liquid-liquid adsorption processes. Other research fields include the development of new methodologies for the high-throughput synthesis of bioactive compounds and preparation of chiral silicon packed-bed microreactors for continuous-flow application.



Dr. Alejandro Cifuentes is a Full Research Professor at the National Research Council of Spain (CSIC) in Madrid. He has been Director of the Institute of Food Science Research and Deputy Director of the Institute of Industrial Fermentations, both belonging to CSIC. Alejandro's activity includes advanced analytical methods development for Foodomics, food quality and safety, as well as isolation and characterization of biologically active natural products. He holds different national and international awards, is member of the Editorial Board of 12 international journals and Editor of TrAC and Electrophoresis. His h index is 38 and his works have received more than 4000 citations (Dic-2012). He has defined for the first time in a SCI journal the new discipline of Foodomics.



Kjell O. Eriksson is senior scientist at GE Healthcare, Uppsala, Sweden. Research area: purification processes, especially in the mAb and recombinant protein area. Defining specifications for new chromatography resins, e.g. user requirements and functional requirements. Characterize downstream processes from an economy perspective. He was research assistant in Uppsala from 1986 to 1990.



Attila Felinger is a Professor of Analytical Chemistry at the University of Pécs (Hungary), in addition to serving as President of the Hungarian Society for Separation Sciences. He graduated with a degree in chemical engineering from the University of Veszprém (Hungary) and obtained his PhD in chemistry in 1988 from the same university; he also holds a DSc degree from the Hungarian Academy of Sciences. His research interests focus on the fundamentals of chromatography including nonlinear, preparative, and analytical separations, as well as the chemometric analysis of measurements by analytical chromatography. Prof. Felinger has published some 100 scientific papers and two books, and serves on the Editorial Board of Journal of Chromatography A, Chromatographia, and LC-GC Europe.



František Foret obtained his PhD in 1991 from the Czechoslovak Academy of Sciences in Brno. He was a postdoctoral fellow with Prof. Barry L. Karger and worked at the Barnett Institute in Boston for additional nine years as a research group leader before returning to Brno in 2001. At present he is a deputy director and head of the Department of Bioanalytical Instrumentation at the Institute of Analytical Chemistry. Since 2011, he is also a group leader at CEITEC Masaryk University in Brno. His main research interests include capillary separations for bioanalysis, miniaturization and mass spectrometry coupling - <http://www.biocentex.cz/>.



Attila Gáspár obtained his PhD in chemistry in 1997 at the University of Debrecen. At the beginning he was working on improvements of sample introduction techniques for atomic spectrometry. From 2000, he continued his research on application of capillary electrophoresis for clinical and pharmaceutical analysis. In 2007, he received expertise on microfluidic analytical techniques at CSU, Los Angeles. Recently he is working on developments of chromatographic and electrophoretic systems on microchips.



Stellan Hjertén, who celebrates his 85th birthday, this year, was born in Forshem, Sweden, but most of his life bound him to Uppsala. His PhD was assigned to him in 1967, and since 1969, when he obtained the professorship, he is actively working at Uppsala University. His broad research work, starting from *hydroxyapatite chromatography*, to the *artificial antibodies* cannot be simply summarized. During his rich research line he invented,

promoted and developed so many new techniques, terms and theories that nowadays it would be impossible to find a biochemist or analytical chemist, who has never heard about Stellan Hjertén. The introduction of *agarose* in chromatography and electrophoresis, the term *hydrophobic-interaction chromatography*, the *homogeneous gels* (recently called as *monoliths*) are just some examples of his scientific achievements. The development of *free zone electrophoresis* certainly revolutionized the separation science, and since the construction of the first “capillary electrophoresis” equipment one of the most cited work belongs to his name in capillary electrophoresis. For his development of the first capillary electrophoresis system he is considered to be “*The Father of CE*”. Stellan Hjertén has received a number of prestigious awards including: the 1985 Björkén Prize (the highest award of Uppsala University) for the development of novel electrophoretic and chromatographic separation methods; the 1988 Electrophoresis Society Founders’ Award for outstanding contributions to the field of electrophoresis, both in practice and theory; the 1993 Frederick Conference Award; the 1993 Bio-Rad Award; the 1994 Hirai Prize (Japan); recognition at HPCE 1996 for distinguished contributions to the field of capillary electrophoresis; the 1996 American Chemical Society National Award in Chromatography; the 1996 Torbern Bergman Medal; the 2001 Pierce Award in Affinity Chromatography and Biological Recognition; the 2002 Golay Award for pioneering work in capillary electrophoresis; and the 2004 Rudbeck Prize for distinguished and internationally appreciated research on methods for the separation of proteins. In 1999, Dr. Hjertén became Doctor Honoris Causa at the University of Pécs, Hungary and was given the same honor at the Vitautas Magnus University, Kaunas, Lithuania in 2001. In 2003, he received the Medal of Faculty of Science at University of Pécs.



Tamás Janáky I have been working for almost 40 years at the University of Szeged, Hungary. At the Endocrinology Laboratory we have developed many radioimmunoassay methods for the determination of peptide, protein and steroid hormones to investigate patients with different hormonal diseases. As a visitor scientist I've spent three years in New Orleans with Nobel laureate Andrew Schally. During that time we have synthesized, analyzed and tested more than 100 LH-RH and somatostatin hormone analogs with anticancer activity. About 20 years ago we have established an Analytical Laboratory at the Department of Medical Chemistry in Szeged, Hungary for the analysis of natural and synthetic peptides with chromatography, capillary electrophoresis and mass spectrometry. Expanding our interest towards the analysis of larger biopolymer proteins, we turned to proteomics and in the last 15 years we have developed new proteomic methods and performed analysis of many samples from bacteria to human tissues. A new 'omics' field, lipidomics is in the focus of our recent research: we are interested in changes of lipidome in different neurodegenerative and oncological diseases.



Ferenc Kilár was born in 1953. He finished his studies as a chemist in 1977 at Eötvös Loránd University, Budapest, Hungary. He started to work at the Institute of Enzymology, Budapest, and then he moved to Pécs, where he is working at University of Pécs since 1983. He received his PhD (CSc) in 1986 and the degree of Doctor of Science in 1995. He was a visiting scientist in Uppsala, Sweden at the Department of Biochemistry, more than 5 years. He took part in the development and application of capillary electrophoresis, mainly using this technique in protein research. In 1997 he was appointed to be a full professor and since then he is the Head of the Department of Analytical Chemistry and Director of the Institute of Bioanalysis, at University of Pécs. Since 2000 he is the Head of the Doctoral School in Chemistry at the University of Pécs. His main research area covers protein-chemistry and the development and application of modern separation methods in bioanalysis. He was a visiting researcher at Università "La Sapienza" and Istituto di Cromatografia, Rome, Italy, University of Bern, Switzerland and L'Institut Pasteur, Paris, France.



Karel Klepárník (1951) is a senior scientist at the Institute of Analytical Chemistry of the Czech Academy of Sciences. In years 1990 - 2001, he was involved in the research and development of capillary electrophoresis for DNA sequencing and mutation detection at the Department of Electromigration Methods. Since 2001, he is responsible for the research of modern analytical methods, mass spectrometry, microfluidic devices and nanotechnologies in molecular biology and medicine at the Department of Bioanalytical Instrumentation. His research interests include theoretical aspects of analytical separations, numerical modeling, mass spectrometry interfacing, laser-induced fluorescence, fluorescence microscopy, surface enhanced Raman spectrometry and analytical applications of micro- and nanotechnologies in single cell analysis. He is the author of over 50 papers in impacted international scientific journals, 2 US patents, 3 chapters in books, 40 lectures (including invited) at international symposia. He received the following scientific fellowships: Institute of Chromatography C.N.R., Rome in 1992, 1994, 2005; The Barnett Institute, Northeastern University, Boston in 1995, 1997, 1999; The Department of Analytical Chemistry, University of Helsinki 2004.



Audrius Maruška graduated from Kaunas University of Technology (1985), obtained there PhD degree in synthesis and evaluation of cellulose adsorbents (1990) and Habilitated Dr. degree at Vilnius University in the field of stationary phases and techniques for microseparations (2002), spent long-term scientific stays at Mainz in the laboratories of prof. Klaus K. Unger, Marburg in the laboratories of prof. Ute Pyell and Uppsala University in the laboratories of prof. Stellan Hjertén. He was elected as a president of Nordic Separation Science Society in 2007 (re-elected in 2009 and 2011). In 2002 in cooperation with colleagues from different universities and Merck, AstraZeneca and Agilent Technologies companies established instrumental analysis laboratories at Vytautas Magnus University. Currently he is the head of a research group at Vytautas Magnus University, which is active in the field of development of microseparations, synthesis of stationary phases, coupling of methods and phytochemical analysis.



Staffan Nilsson Professor, Lecturer Center for Chemistry and Chemical Engineering Pure & Applied Biochemistry, LTH, Lund, Sweden - since 2007.

Main scientific achievements: Purification of biological active membrane-protein 1988; HPLC Protein G 1987; TLAC of protein (pregnancy test) 1992; Real-Time Fluorescence Imaging of CE-separations 1995; Protein based Monolith CEC enantioseparation 1995; MIP based; Monolith CEC enantioseparation 1997; “Wall-less” test tubes for CE 1998; Airborne Cell analysis 2000; MIP nanoparticle PSP-CEC enantioseparation 2000; Ultrasonic trapping in CE 2001; NP-PSP-CEC-ESI/MS 2002; Airborne Chemistry-Protein Crystallisation 2003; Airborne Chemistry X-ray Scattering 2003; \Nano-Spray ESI MS CEC/CE 2004; Levitated droplet dye laser 2006; NACE of EtOH Markers 2008; Monoclonal nanoparticle PSP-MIP-CEC 2008; Airborne Cell-Cell communication 2009; Chip-PSP-CEC 2010; Open Chip SAW-MALDI MS Sample Handling 2012.



Gabriel Peltre has studied biochemistry and immunology at the Paris University. He started his PhD at the Pasteur Institute. His thesis was about the antibody response to a model antigen, an enzyme, in animal models.

After a two years post doc in California he chose to work on allergy, on purification, isolation and identification of molecular allergens. His group became also very interested by the nature, the amount and evolution upon time of the different antibodies to allergens in patients as well as in normal individuals. He was teaching French or International courses in immunochemistry. He developed new techniques of immunodetection following electrophoretic techniques such as immuno-fixation and blotting. He became in 1982 the first president of the French Electrophoresis Society. He had a very active international collaboration.



Melinda Rezeli got her PhD degree in chemistry at the University of Pécs in 2008, with the thesis on the development of acrylamide-based separation matrices. During her postgradual studies she spent two years in the prestigious Stellan Hertén's laboratory at Uppsala University. In 2007 she joined a biotech company in Pécs, Hungary as a researcher and took part in the development of immune-based multiplex assays in the field of life sciences and healthcare. Currently she is working at the Biomedical

Center of Lund University as a research scientist. Her main research interest focuses on mass spectrometry based protein biomarker quantitation, including

multiplex assay development and biomarker discovery. Dr. Rezeli has published 22 scientific papers in international well-recognized journals.



Johan Roeraade was born in 1942, and has been active in research for almost 50 years. He has been engaged in almost every field of separation science. He was a pioneer in the use of microchips in chemistry- a work which he started for more than 25 years ago, and for which he obtained the Norblad-Ekström gold medal. He has published more than 150 scientific articles and has 20 patents. He has given more than 250 lectures at international conferences. In 2007, he obtained the prestigious A.J.P. Martin Gold Medal for outstanding achievements in separation science. For a long time, his work focuses on biochemical analysis, and his recent work in mass spectrometry was awarded with the Beynon Prize at the ASMS in 2012. Johan Roeraade is now a prof. emeritus, but he is still a very active researcher at his former department of Analytical Chemistry at the Royal Inst. of Technology in Stockholm, where he has been for more than 30 years.



Zoltán Szőkefalvi-Nagy studied physics at the Eötvös Loránd University in Budapest and obtained his PhD in nuclear physics in 1970 and the degree Doctor of Science in 1993. He is working in the Central Research Institute for Physics of the Hungarian Academy of Sciences and its successor institution since 1967. In 2003-2011 he was the director of the KFKI Research Institute for Particle and Nuclear Physics (in 2012 the institute became the part of the MTA Wigner Research Centre for Physics.) Now he is research professor emeritus in this Centre. As an invited professor he is teaching Biophysics in the Faculty of Veterinary Sciences of the Szent István University since 1995. His research activity is all along connected to the Van de Graaff accelerator. His main research interest is the use of ion beam analytical (IBA) techniques in various interdisciplinary problems. He made important achievements in the elemental analysis of proteins, He invented the PIXE-PAGE method by combining the particle induced X-ray emission spectroscopy with thin layer electrophoresis. His results in non-destructive analysis of cultural heritage objects are also internationally recognized. In 2007 he got the Simonyi Károly Award.



Dr. Thierry Tron is 49 years old, Principal Investigator at ISM2 UMR7313, Aix-Marseille University Doctor of the University of the Mediterranean (currently Aix-Marseille University). Between 1987-1991, he was a PhD Student, University of the Mediterranean (France), in the group of Dr. D. Lemesle-Meunier and Catholic University of Louvain (B), and he worked in the group of Pr. A. M. Colson with an EU mobility fellowship. In 1991, FEBS Postdoc

fellow (3 months), at University of Bologna, in the group of Dr. M. Degli Esposti, and an FRM Postdoc fellow (7 months), at CNRS Marseille. Between 1992-1994, he received a HFSP Postdoc fellowship at Dartmouth Medical School (USA), in the group of Pr. B. L. Trumpower. Between 1994-1998, researcher, at Aix Marseille University. Since 1999, he is senior researcher and group leader, at ISM2 UMR7313, Aix Marseille University. Other professional experiences: Direction of a research group of 2 CNRS researchers and 1 associate professor; Direction of 6 PhD theses, responsibility for 4 post-doctoral associates; Involvement in 3 ANR (1 as a coordinator) and 2 EU projects since 2004. His research interest is metalloenzymes and artificial metalloenzymes. Publications: 30 papers in international journals (total citation: 508, h-index: 12), 1 patent, 2 book chapters.



Ákos Végvári is an associate professor and senior research scientist at Lund University. He was born in Siklós, Hungary, in 1968. He got his degree in Biology in 1996 at the University of Pécs, Hungary, with a thesis on the bioanalytical applications of capillary electrophoresis. During the period of 1997-2001 and 1999-2003, he received PhD degree in analytical chemistry at the University of Pécs and PhD degree in biochemistry at the Uppsala University, Sweden, respectively. He has worked on analytical methodology development for separation of peptides, proteins, and nucleic acids. He joined a biotechnology company in Stockholm, working on the analytical evaluation of a newly developed AIDS drug. He is currently working at the Biomedical Center of Lund University. His main research interests focus on disease linked, mass spectrometry based proteome analysis, including targeted cancer proteomics as well as fundamental method development for localization of drug compounds in tissue sections by MALDI imaging mass spectrometry. Dr. Végvári has published more than 45 scientific papers within internationally well-recognized journals and has written five book chapters. He has an h-index of 14 and a total of 600 independent citations.

Abstracts

Doctoral Forum

DF-01

COMPARISON OF OVERALL MASS-TRANSFER COEFFICIENTS OF SUPERCRITICAL FLUID CHROMATOGRAPHY AND LIQUID CHROMATOGRAPHY

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Abstract

A number of equilibrium and kinetic macroscopic models are used to understand the chromatographic processes in liquid chromatography [1]. These models, however, cannot be used easily to characterize the mass-transfer in supercritical fluid chromatography (SFC), due to the variation in the physico-chemical properties of the mobile phase along the column.

The stochastic model of chromatography describes the separation process as a random migration, and randomly occurring adsorption-desorption of the molecules in the chromatographic column [2]. According to this model, the number of adsorption and desorption steps and the sojourn time that a molecule will spend on the stationary phase during the adsorption are random variables. By using the first and the second central moments of the chromatographic peaks, the mass-transfer coefficients can be calculated [3].

In this study the first and the second moments of alkyl-benzene peaks - measured on the same column in UHPLC and SFC systems - were used to explore the differences in the mass-transfer processes between the two chromatographic modes.

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DF-02

INVESTIGATION OF THE RETENTION PHENOMENA OF MEFLOQUINE ENANTIOMERS: EFFECT OF THE ELUENT COMPOSITION

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Abstract

A cinchona alkaloid-based zwitterionic chiral stationary phase (ZWIX) was applied for enantiomer separation of rac-erythro-mefloquine. A Chiralpak ZwiX(+) analytical column was used for the separation. The overloaded peak profiles have confirmed that there is significant difference between the adsorption-desorption phenomena of the two enantiomers. Whereas the 11R, 12S enantiomer shows a strong retention and a common BiLangmuir behavior, the 11S, 12R enantiomer has a weak retention near to the column void time. The weak retention phenomenon is most probably caused by the repulsive interactions between the analyte and the CSP (chiral stationary phase). These repulsive effects, which are mostly polar and hydrogen-bonding interactions, can be modified by changing the eluent composition. The purpose of the present work is to vary the methanol-acetonitrile-water composition and the buffer ratio of the applied eluent. The first results show that it is necessary to use a small amount of buffer. On the other hand, increasing the level of the aqueous phase in a buffered organic eluent, decreases the selectivity (α), although better peak shapes can be obtained.

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DF-03
**MODELING WIDE PORE SIZE DISTRIBUTIONS IN SIZE EXCLUSION
CHROMATOGRAPHY**

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Abstract

Chromatographic processes can easily be modeled at a molecular level using the characteristic function approach. This model is completely independent of the physical chemical mechanisms responsible for the retention; therefore it can be used for any chromatographic process such as adsorption, partition, ion-exchange or size exclusion chromatography.

The size exclusion process is pictured as the molecules of the same size enter the pores of the stationary phase n times on average, and spend in a pore time τ_s on average. After leaving the pores, the molecules spend time τ_m on average in the mobile phase. Each molecule has an individual path in the column, but because of their same size and behavior, the average time the molecules spend in the column will be t_R and the chromatogram will be nearly a Gaussian curve.

The characteristic function of the band profile in SEC was described earlier by Dondi et al [1]. The moments of the chromatographic peak can be derived from the characteristic function. However, the retention of the macromolecules rises from both the hydrodynamic chromatography effect and the size-exclusion effect. The retention of the excluded samples comes only from the hydrodynamic chromatography effect. The original model assumes that the pore sizes in the column are equal in each stationary phase particle.

In this work, we assume that the pore size in the stationary phase of chromatographic columns is governed by a wide lognormal distribution. This property was integrated into the molecular model of SEC and the moments were calculated for several kinds of pore shape.

Our results demonstrate that wide pore size distributions have strong influence on the retention properties (retention time, peak width, and peak shape) of macromolecules. The novel model allows us to estimate the real pore size distribution of commonly used HPLC stationary phases.

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DF-04

COMPARISON OF BIOSORPTION PROCESSES BY BACTERIAL AND ALGA CELLS

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Abstract

Heavy metal pollution is one of the most important environmental problems. Heavy metals, such as cadmium, lead, copper and zinc can cause serious health hazards. Their presence in soils, natural and drinking water can be harmful even at low concentrations. Natural materials of biological origin, including bacteria, fungi, yeast and algae possess metal-sequestering property and can be used to decrease the concentration of heavy metal ions with high efficiency and quickly. These biosorbents are an ideal candidate for the treatment of high volume and low concentration complex wastewaters containing heavy metal ions.

The aim of this study is to compare the biosorption characteristics of different microorganisms: 4 bacteria and 3 algae. These are *Pseudomonas aeruginosa* and *Pseudomonas fluorescens*, *Escherichia coli* and *Escherichia coli D31*, *Chlorella pyrenoidosa* and *Spirulina platensis-Spirulina maxima* mixture. The results will be given concerning to activated carbon, because many water purification technologies are using it. The effect of pH, temperature, initial metal concentration and adsorption time on bioadsorption was studied. The residual metal content of the solution was determined using flame atomabsorption spectrophotometer (AAS).

DF-05

MODIFIED, LAYER COATED AMPEROMETRIC SENSOR FOR MEASURING IN NATURAL, POROUS MATRICES

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Abstract

In voltametric analysis the current resulted by electrode reaction of the analyte is used for evaluation. In optimal cases the current is determined by the diffusion mass transport of the electroactive analyte. Well known basic equations relating to different voltametric methods like the Cottrell, the Randles-Sevcik, the Ilkovic, or the Levich equations show that well defined linear dependence exists between the current and the analyte concentration. Therefore in voltametric analysis calibration curves are used for evaluating the concentration of sample solutions. Evaluation with the calibration data can result in accurate concentration value as long as the diffusion coefficient of the detected species is the same in the standard as in the sample solution. However, if it is not the case, then the calibrating data obtained with the standard solution can not be used for obtaining reliable concentration values. Adding small volume doses of standards to the sample would not change much of the diffusion character. The so called standard addition method takes advantage of this. There are special analytical tasks where neither the standard addition methods nor diffusion property harmonizing standard can be applied. Examples for this can be analysing electroactive species in extracellular space of tissues of living animals, or plants. Furthermore this kind of special tasks can be measuring concentration of electroactive species in other tortuous matrix like in fruits or in sediments. In our recent studies a way for solving those special analytical tasks with voltametric technique has been worked out. The method employs short time chronoamperometric data collection and a special modified working electrode type. The electrode is modified with a thin diffusion layer coating its surface. Doing the measurements the built in diffusion layer at the electrode surface is equilibrated with the sample or with the standard solutions. Appropriate constant measuring potential is applied for a few seconds and the current – time transient is recorded. As the electrode reaction proceeds, the concentration of the detected species decreases in the vicinity of the electrode. Short time after the electrolysis started the diffusion profile is inside the built in diffusion layer. Therefore we can use the short time current values recorded in aqueous calibrating standards for evaluating short time chronoamps recorded in special standards. The lecture will show the preparation of the electrode using vitamin C and iodine as analyte, sand sediment, and green pepper as model matrix.

DF-06

PRELIMINARY RESULTS FOR THE STABLE ISOTOPE COMPOSITION OF LATE PLIOCENE ENVIRONMENT IN FOSSIL *STEPHANORHINUS* SP. AND *MAMMUT* SP.

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Abstract

The study is focused on the Late Pliocene paleoclimate and habitat paleoecology. Oxygen and carbon isotopes are analyzed in mammal skeletal apatite. The study material consisted predominantly of fossil teeth of the *Stephanorhinus* KRETZOI 1942 (rhinoceros) and *Mammut* BLUMENBACH 1799 (mastodon), collected from the Carpathian basin, almost entirely from Hungary. According to biostratigraphy the ages of samples range from 3.5 Ma to 2.0 Ma. Altogether 20 specimens were sampled for the isotopic work. The $\delta^{13}\text{C}$ are determined of structural carbonate in the bioapatite component. The ^{18}O analyses are followed a preparation technique adapted after Kocsis [1]. The cleaned samples are dissolved in HF and the obtained solutions neutralized (25% NH_4OH), followed by rapid precipitation of Ag_3PO_4 . After drying at 70°C , the silver-phosphate will be analyzed via reduction with graphite in a TC/EA (high-temperature conversion elemental analyzer) [2] coupled to a Finnigan MAT Delta Plus XL mass spectrometer. International NBS-120c phosphorite rock standard are prepared and run together with the samples. The oxygen isotope composition of the precipitating skeletal apatite is determined solely by the isotopic composition of the animal's body water [3]. The $\delta^{18}\text{O}$ values will be determined in the bioapatite phosphate. The results of the oxygen isotope analysis of rhinoceros and mastodon enamel phosphate will provide the first estimate of $\delta^{18}\text{O}$ values in Late Pliocene and Early Pleistocene precipitation in Hungary. The isotopic composition of carbon in the enamel samples will indicate the diet for the Hungarian rhinoceroses and mastodons, in comparison with previous investigations of Late Pliocene ecology.

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DF-07

A STUDY OF ZINC BINDING TO CASEIN IN LIGHTS OF POTENTIAL MEDICAL APPLICATIONS

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Abstract

Casein is the main protein of milk and the most useful building block for the synthesis of hemoglobin and plasma proteins. It is a phosphoprotein, which forms residues of ortho- and pyrophosphate, ester-linked to monoesters or diesters - molecules at specific sites - mainly serine, and threonine. The main fractions of casein are: α , β , γ . Casein is used as a dietary supplement designed for athletes. Its unique properties of gel formation are widely used in the production of cheeses, and also serves as a filler. In milk, casein occurs mainly in the form of micelle. Casein micelles are formed from subunits consisting of individual fractions of casein monomers linked together by a bridge formed by calcium ions, phosphate, and citrate.

Zinc cations are present in many centers of active enzymes involved in metabolism. They participate in bone mineralization, wound healing, they have an effect on the immune system, normal secretion of insulin by pancreas, and on concentration of vitamin A and cholesterol. They also contribute to regulation of blood pressure and heart rate. However, the major problem is assimilation of zinc cations in the body. Zinc deficiency causes anemia, slow growth, birth defects, poor wound healing, psoriasiform skin lesions, dermatitis and hair loss, poor glucose tolerance. Zinc is a healing for stomach ulcers, persistent varicose veins, arthritis, ulcers, acne, skin diseases. Synthesis of zinc metalloproteins based on casein creates a potential application in the field of medicine. In this case explanation of the processes and mechanisms of binding zinc to casein is very important. Obtaining stable metalloproteins is an essential step in the process of their research and potential application: antiseptic and dietary supplements. In addition, stable complexes of metalloproteins will serve as an indispensable tool in the study of metal cations transfer mechanisms in living cells of eukaryotes and prokaryotes. Knowledge about mechanism of zinc binding with the proteins could be used as a tool in their possible medical application [1-3].

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DF-08

KINETICS AND MECHANISM OF THE PENTATHIONATE-IODINE REACTION

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Abstract

Pentathionate has been confirmed to be one of the important sulfur-containing intermediates and may contribute to the appearance of a rich variety of kinetic phenomena during oxidation of thiosulfate[1–3]. Studying the oxidation of pentathionate may contribute to a better understanding of the oxidation of other polythionates and the mechanistic studies of the oxidation of thiosulfate. In this lecture, we present the results of our investigations on the pentathionate-iodine system. The reaction can easily be followed by UV–visible spectroscopy and, on the other hand, the kinetics of trithionate-iodine[4] and tetrathionate-iodine[5] have already been available for comparison. It was found that pH does not affect the rate of the reaction, however, iodide ion, produced by the reaction, strongly inhibits the oxidation, therefore it acts as an autoinhibitor. The same kinetic phenomenon was also observed in the other polythionate-iodine reaction. The kinetic curves also support the fact that iodide inhibition cannot be explained by the formation of the unreactive triiodide ion, and $S_5O_6I^-$ along with iodide ion have to be involved in the initiating rapid equilibrium shifted far to the left. Further reactions of $S_5O_6I^-$ including its hydrolysis and reaction with iodide ion lead to the overall stoichiometry represented by the following equation: $S_5O_6^{2-} + 10I_2 + 14H_2O \rightarrow 5SO_4^{2-} + 20I^- + 28H^+$. A nine-step kinetic model with two fitted parameters is proposed and discussed from which a rate equation has also been derived. A short discussion about the general pathway of sulfur-chain breakage of polythionates has also been included.

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DF-09
**ELECTROPHORETIC AND MASS SPECTROMETRIC ANALYSIS OF
BACTERIAL ENDOTOXINS**

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Abstract

Lipopolysaccharides (LPSs, or endotoxins) are the main components of the external membrane of Gram-negative bacteria. LPS is composed of three distinct structural regions: the O-chain polysaccharide, the core oligosaccharide and the lipid A moiety. Lipid A serves as the hydrophobic anchor of LPS in the outer membrane and is mainly responsible for the endotoxic activity. It generally consists of a β -1,6-linked glucosamine disaccharide backbone that is acylated by up to seven C10-C18 fatty acids or β -hydroxy-fatty acids linked as ester at C3 and C3' positions and as amides at C2 and C2' positions. The hydroxyl groups of these β -hydroxy-fatty acid chains can be further esterified by additional fatty acids. Phosphates, with or without other substituents, are linked at C1 and/or C4' positions. The number and type of the acyl chains and the state of the phosphorylation of the glycolipid are fundamental determinants of the toxicity of LPS.

The structure of lipid A is relatively conserved compared to the highly variable O-chain polysaccharide. The lipid A samples from a single bacterial population may contain more than one lipid A structural type, as well, partial or incomplete structures as a result of incomplete biosynthesis. The moderate variability of lipid A molecules might serve as the basis for the rapid identification of bacterial strains.

A comprehensive study was continued to develop phosphoglycolipid profiling techniques determining the acylation and phosphorylation pattern of lipid A extracted from several bacterial strains. Mass spectrometry (MALDI-MS, ESI-MS) itself, and hyphenated with capillary electrophoresis were used in the structural elucidation of intact LPSs and lipid A moiety.

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Abstracts

Lectures

L-01

THE ARTIFICIAL COUNTERPART OF THE NATIVE PROTEIN ANTIBODY

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Abstract

During the last 4-5 years I have devoted much time to develop a novel, patented, general theory of interactions in non-living, as well as in living systems, based on only two well-defined parameters, which can easily be experimentally determined: net surface hydrophobicity (by HIC on *neutral* matrices) and negative net surface charge (by Free Zone Electrophoresis).

I introduced these two methods in the seventies.

When the latter parameter has the value zero, another theory is valid: that of the protein antibodies in living systems, which is identical to my theory of the artificial gel antibodies in non-living systems, I introduced almost 20 years ago [1]. I will discuss the theory of these gel antibodies and some of their applications. Several of the experiments I will refer to in my lecture were performed in collaboration with Prof. Ferens Kilár and his collaborators.

A third theory obtains when the net surface hydrophobicity=0. This theory is applicable to interactions, for instance where nucleic acids are involved, including their interactions with the enzyme DNase.

My lecture will be centered around the second theory above, illustrated with several applications.

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L-02

IDEAS, TRIALS AND PROGRESS IN THE ANALYSIS OF LOW-ABUNDANT BIOMOLECULES

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Abstract

Analysis of biomolecules, occurring at ultra-low concentrations in body fluids must be considered as the most challenging task for the analytical chemist. This is partly due to the chameleonic behavior of such molecules, but also due to the presence of an excessive number of compounds with a similar behavior. Methods, based on specific immuno-affinity have long been the standard tool to solve such problems, but these are not always reliable when dealing with very low-abundant components.

The great potential of combining immuno-methods with miniaturized separations and sensitive detection methods will be outlined in this lecture. This includes some new ideas for separations as well preparative fraction collection from CE-columns, followed by MALDI-TOF MS, and the use of ultra-miniaturized MALDI-targets, combined with handling of picoliter sized volumes. With the latter technology, we have been able to obtain a consistent limit of detection down to 10 zeptomol. for a number of model peptides.

We have utilized the outlined technologies for the analysis of A β -peptides in cerebrospinal fluid as well as in blood plasma. These peptides play a major role in the development of plaque in the brain, causing Alzheimer disease. Compared to conventional protocols, our results indicate that we have at least a hundred-fold improvement in limit of detection.

L-03

DIVERSITY OF ALLERGENS AND OF THE ANTIBODIES RAISED TO THEM, A CHALLENGE FOR BIO ANALYTICAL METHODS

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Abstract

Allergy is a widespread disease which is touching 15 to 30 % of the population, mainly from the developed countries. The number of allergy cases has doubled in the last 15 years. Diagnostic and therapy are still performed by using highly heterogeneous crude extracts of allergenic sources. A new trend is now in development: the replacement of these ill-defined mixtures by purified extracts, single allergenic molecules or even recombinant allergens.

Allergens are mainly proteins. From one natural allergenic source, for example a pollen extract, 10 to 20 single molecules can be recognized as allergens by patient sera. To study the allergen repertoire, or allergome, the best technique used so far consists in a proteomic approach: a 2 dimensional separation of the crude extract in polyacrylamide gel followed by an immunoblotting detecting the allergens as the molecules bound to IgE antibodies from a patient serum.

Antibodies to single allergens are also highly heterogeneous. Little is known about their role in the disease. The pathologic antibodies, responsible of the allergic symptoms are IgE antibodies present in minute amounts, in the ng/ml range, in the blood. The presence of IgGs, present in a concentration 1000 times higher as a mean, is usually the sign of the allergenic sensitization of an individual. IgM and IgA are also found in fair amounts in patient sera. The presence of auto anti IgE antibodies has been reported and increases further the complexity of the allergen specific antibody response.

Diagnostic of allergy is mainly based on clinical tests, the manifestation of allergic symptoms. The gold standard of the in vivo diagnostic tests is the skin prick test. In vitro allergy tests have been developed based on the allergen specific IgE antibodies present in patient sera. The concentration of these antibodies is not directly proportional to the severity of the allergic symptoms. Even 10 % of the persons who have positive IgE values do not suffer from allergic symptoms.

Therapy needs more and more the use of well defined molecules to trigger the immune system and induce a protection based on allergen specific antibodies. Recombinant allergens are certainly a good answer to these needs

Conclusions. Allergy is a very common disease. A lot is still to be understood in its induction and its evolution upon time. It may act as a good model for the treatment of other more dramatic diseases induced against complex molecular mixtures such as viral or parasitic infections.

THIN METAL LAYERS IN BIOANALYSIS

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Technology developments in the few past decades have created opportunities for multidisciplinary research combining materials science, electronics and chemistry. Although consumer electronics has thus far had the most significant influence both on the economy and culture, the underlying technology creates a strong potential also in new areas of chemistry. Thin film deposition technology, a routine part in the production of most electronic and optic components, is finding its ways into new areas of chemical and biochemical sensors and instruments. At present the thin layers of metals serve in applications spanning from simple electrodes to surface plasmon resonance (SPR) or giant magnetoresistance (GMR) based sensors. Thin films allow monitoring redox processes in the vicinity of electrodes, adsorption/desorption equilibria of ions, organic compounds, gases, and more recently also interactions of large organic macromolecules such as proteins or DNA. Measurement of basic photonic and electric properties (current, voltage, resistance) is simple with large dynamic range. In this work we focus on the development and applications of thin metal films with the submicron thickness for surface sample enrichment and detection based on electrochemiluminescence, surface reflectivity and resistance changes. We shall discuss the potential of thin metal layers for chemical sensing and reversible chemisorption for sample sensing and enrichment on a microscale.

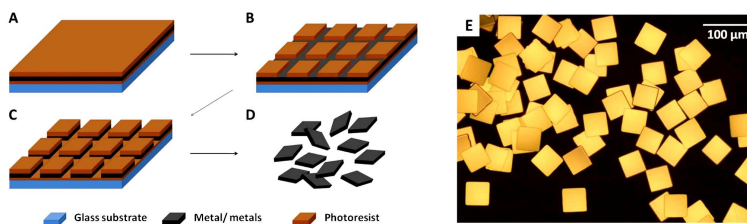


Fig. 1 Preparation of structured metal particles with submicrometer thickness.

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A METABOLOMIC STUDY OF THE ANTIPROLIFERATIVE EFFECT OF CARNOSIC ACID AGAINST HUMAN COLON CANCER CELLS**C. Ibáñez, A. Valdés, V. García-Cañas, C. Simó, A. Cifuentes****Laboratory of Foodomics, CIAL (CSIC). Nicolas Cabrera 9,
28049 Madrid, Spain (a.cifuentes@csic.es)***Abstract**

Safety, quality and bioactivity of foods and food ingredients are investigated in Foodomics through the application and integration of advanced omics technologies, including genomics, transcriptomics, proteomics and/or metabolomics. The main goals of Foodomics are to improve consumers' well-being and knowledge [1-3].

Based on a recent work from our group, in which a global Foodomics study was performed to investigate the antiproliferative activity of different extracts from rosemary against colon cancer cells [4], we present in this work an step forward in this long investigation in which a complete metabolomics study (combining results from LC-MS and CE-MS platforms) is carried out to corroborate the antiproliferative effect of one of the main dietary polyphenols that was found in all the active rosemary extracts (i.e., carnosic acid). Moreover, the present work provides additional information on how this polyphenol from rosemary is able to modulate a specific metabolic pathway in the colon cancer cells (i.e., polyamines pathway), providing new evidences at molecular level on the antiproliferative effect of this type of compounds.

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LIPOPOLYSACCHARIDOMICS – A COMPLEX APPROACH

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Abstract

Lipopolysaccharidomics is an emerging research area that covers the large-scale analysis of bacterial lipopolysaccharides (LPSs). These molecules (also called as endotoxins) are physiologically active components of the outer membrane of gram-negative bacteria and are released during growth, division and lysis. They have been recognized as the most potent stimulants of mammalian immune systems, causing a wide spectrum of pyrogenic and toxic reactions. LPS consists of a lipid region, termed lipid-A covalently attached to a polysaccharide region. Both regions have extremely high variability in their structures, which directly affects their physiological impact. Though several methods have been used for endotoxin analysis, much progress is still needed to separate and identify the many subclasses and clarify the structure-function relationship of LPSs from individual strains. The essential problems faced in LPS research are i) the amphipathic, ii) non-UV-active and iii) intrinsic heterogeneity of LPS molecules. A comprehensive study was continued to explore the complex structure of the components with several unique sugar components and differences in the lipid part [1]. The novel and fast methods using conventional capillaries and microchips with LIF detection developed especially for endotoxins allows 1) to differentiate between R and S endotoxins, 2) to monitor endotoxin-protein complexes and 3) determine the molecular components of the toxic variants. MALDI-TOF MS, GC-MS and CE-MS studies were conducted to prove the presence of the different molecular forms, including the “absolute R”, this form together with the “core”, which contained unusual heptose units, and also the repeating units that are responsible for toxicity and immunogenicity. The techniques developed are usable to analyse and confirm the structures and types of LPSs directly from the cell cultures of the bacteria. This is of high importance, when fast analyses are necessary in infection and in preparation of human vaccines.

Acknowledgements

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L-07

DRUG LOCALIZATION IN TISSUE SECTIONS BY MALDI-MS IMAGING

Ákos Végvári

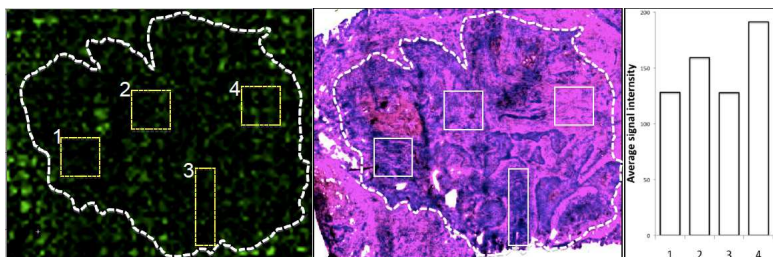
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Abstract

New drug characterization assays are essential for providing evidence to the specificity and selectivity of drugs. Technological developments offer a novel tool to achieve highly detailed spatial information in tissue compartments at 10 μm spatial resolution by MALDI mass spectrometric imaging. Although the intensity of a given mass signal is influenced by many factors, the visualization of m/z values in two-dimensional space specifies an image corresponding to certain histological compartments.

Basic physical and chemical properties of drugs in different tumor phenotypes were analyzed in experimental arrangements that form the basis for rodent models, characterizing drug distribution kinetics. Reduced compound signals could be associated with tumor regions, particularly in the squamous cell phenotype due to the large size areas of tumor cells [1]. Sample preparation of the tissue prior to analysis is of importance and pre-solvatization of the tissue is recommended. The specific experimental conditions are needed to be optimized for any given tissue type [2].

The benefit of the high spatial resolution can provide close match to the corresponding high-resolution histology scans, allowing queries of mass spectra at precise locations in the specimen [3]. Instrumentation, analytical principles, experimental models and case studies will be presented to demonstrate the capabilities of MALDI mass spectrometry imaging.



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Recently, the focus of proteomics studies has been transferred to quantitative aspects, although quantification of peptide and protein biomarkers in complex biological matrices, such as human plasma, is a challenging task [1]. Despite the continuous technological developments the diagnostic value of the newly discovered biomarker candidates is limited. Inadequately controlled sample collection/sample handling is probably one out of the several reasons why these candidates are not able to deliver on those preliminary expectations, which for instance relate to clinical diagnosis in modern health care. Inventories of high quality clinical samples are prerequisite for designing the next generation diagnostics and treatments for patients. Disease presentation and clinical sample collection are key strategic resources that can provide new insight and understanding of disease mechanisms.

In biomarker discovery at the verification and the validation phase, the determination of the levels of high number of candidate biomarkers in different body fluids in large sample sets is crucial in future health care developments. The requirements are rigorous: as the assay must be sensitive, accurate, and highly reproducible while the high throughput is also an important aspect. Currently, the highly sensitive and specific immunoassays are commonly used for verification and validation of new biomarkers, although mass spectrometry-based targeted approaches, such as selected reaction monitoring (SRM; or MRM in plural) with stable isotope dilution strategy, allow accurate quantitation and provide an alternative method to antibody-based approaches [2]. SRM is a targeted MS-based technique, generally performed on triple-quadrupole (QqQ) instruments. MRM assays provide good sensitivity and quantitation of proteins/peptides in a broad dynamic range [3].

We worked in close collaboration with different clinical groups, and developed multiplex, mass spectrometry-based quantitative assays. The assays were utilized for screening of biobanking materials, and performed comparative analysis of patient groups in various disease areas, such as cardiovascular diseases, neurodegenerative diseases and cancers.

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L-09

INCREASED BIOLOGICAL VALUE AND SAFER FOOD PRODUCT DEVELOPMENT USING SOLID STATE FERMENTATION OF PLANT MATERIAL WITH BACTERIOCINS-PRODUCING LACTIC ACID BACTERIA: COMPARATIVE PHYTOCHEMICAL ANALYSIS OF FERMENTED AND NON- FERMENTED SAMPLES

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Abstract

Medical plant raw material (collected at Vytautas Magnus University, Kaunas botanical garden, medicinal plants sector) have been studied before fermentation and after various fermentations with lactic-acid bacteria and yeast. Fermented samples and ground raw material were obtained from Kaunas University of Technology. Medicinal plants rich in phenolic compounds and essential oils and plant protein products - flax seeds have been studied. According to radical scavenging activity, phenolic compounds and flavonoids content before and after fermentation, the tested plants can be divided into two groups: (I) plants in which fermentation significantly decreases the total phenolics and flavonoids content (by 2-3 times), but the scavenging activity of free radicals is not decreased or even increased; (II) plants that after fermentation has not significantly increase in total phenolics and flavonoids content and radical-scavenging activity does not change or increases significantly. Volatile compounds of medical plant material have been analyzed before and after fermentation, the dynamics of the different compounds, using various lactic acid bacteria and yeast fermentations have been evaluated. All the identified compounds can be divided into three groups: (I)-compounds which present in fermented and non-fermented samples (II) - new compounds that occur during fermentation and (III) - compounds that are not determined after fermentation. All of these variations both in terms of quantity and quality depend upon the plant and fermentation microorganisms used.

Acknowledgement: Financial support from Lithuanian Science Council Fund (Grant No. SVE-09/2011 **BIOFITAS**) is acknowledged.

L-10

DEVELOPMENT OF INTERMEDIATE PURIFICATION STEP IN INSULIN PROCESS USING A HIGH THROUGHPUT APPROACH

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Abstract

Designing a purification step for a complex target molecule is challenging as the tentative combinations of conditions and chromatography media (resins) are many. One of the responses of major interest in an intermediate purification step is selectivity. This presentation will focus on the methodology used to design a step that follows on enzymatic cleavage of pro-insulin into main product, insulin, and the C-peptide.

In order to speed up process development and keep sample amounts low it is advantageous to use a parallel format with low resin volumes. The 96-well batch format meets these demands and was used to screen for most promising resins and conditions, both with respect to yield and purity. The knowledge gained from an elution study utilizing 20 µl resin per well, followed by optimization in small columns, was scaled up to a 400 mL column scale intermediate purification of insulin to more than 90% purity.

L-11

SINGLE CELL ANALYSIS: STATE OF THE ART

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Abstract

Single cell analysis (SCA) can potentially play an important role in the systems biology, where biological processes in terms of interactions of molecular components are studied at different molecular levels, from genome to cellular function. With respect to this, analyses of individual cells or even the cell organelles may offer unique information on differentiation, specialization, proliferation, senescence and cell death. Moreover, SCA can reveal an effect of cell-cycle, different life conditions, and surrounding environment on the genome, transcriptome, proteome, peptidome and metabolome of a cell.

The following data demonstrate the demands exerted on this type of analyses. The total mass of a typical eucaryotic somatic cell of a diameter of 5 - 10 μm and a volume of ~ 0.5 pl is about 500 pg. Only 10% of the cellular mass form about 2 fmol of about 10 000 various expressed proteins. Among them, about 200 zmol or $1.2 \cdot 10^5$ copies represent medium abundant proteins, only about hundreds of molecules of cellular receptors, $10^3 - 10^4$ of various signaling enzymes and 10^8 molecules of structural proteins.

In this talk, more than a quarter of century long history of SCA will be overviewed. Throughout this period, it has been demonstrated that miniaturized capillary or microfluidic devices furnished with advanced detection methods provide suitable conditions for the analysis of chemical content of individual cells, cell organelles or even detecting single molecules. The recent development of nanotechnologies brings new extraordinary opportunities into the practice of analytical chemistry. The combination of specific probes, labels and sensors with powerful and stable light sources, advanced optical arrangements and high-sensitivity detectors allows detecting and tracking even single molecules with nanometer spatial precision and millisecond time resolution in living cells.

ENGINEERING LACCASES: IN SEARCH FOR NEW BIOCATALYSTS

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Abstract

Laccases are very well known biocatalysts with great robustness, high oxidation power and substrate versatility (among other properties) [1]. They contain a unique set of copper ions made of one each of the three types of biorelevant copper sites: type 1 (T1), type 2 (T2) and a binuclear type 3 (T3), and couple dioxygen reduction to the oxidation of substrates, either organic or metal ion [2]. They belong to the Blue Copper Binding Domain (BCBD) family of proteins in which the archetypal members are the plant or bacterial electron transfer protein cupredoxins (CUP). In this family, function is modulated by the number of CUP domains, the number and type copper atoms and the fusion to non metallated domains. Taking natural plasticity within the BCBD family as a source of inspiration for the engineering of laccases [3, 4], we aim at shaping new catalysts based on a laccase platform **functionalized** with “plug-ins”.

One of our targets is to develop a robust system where light absorption triggers electron transfer from a catalytic centre to a renewable electron acceptor. We report here on the light driven four-electron reduction of a laccase that ultimately converts dioxygen into water using ruthenium(II) polypyridine or porphyrin type chromophores and a sacrificial electron donor [5]. Prospects of development of renewable aerobic photo oxygenation catalysts will be presented.

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L-13

IDENTIFICATION PEPTIDES AGAINST ALZHEIMER'S DISEASE: A PROTEOMIC APPROACH

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Abstract

Alzheimer's disease (AD) is the most prevalent form of neurodegenerative disorders. Recently, it is widely accepted that oligomeric amyloid-beta peptide (A β) toxicity may be responsible for the initiation of AD. Interaction of A β with proteins is the key event in the pathology of Alzheimer's disease. Mapping the A β interaction partners could help to discover novel pathways in disease pathogenesis and to find targets for drug development.

The aim of our research was to discover small peptides inhibiting the interaction of these proteins with A β .

Our proteomic studies have revealed that the fibrillar A β (1-42) peptide binds to a huge number of proteins derived from rat synaptosomal membrane fractions. Majority of these identified proteins have already been associated with Alzheimer's disease.

The protein array technology is a novel method to investigate protein-protein interactions in a high-throughput manner. To investigate the potential interaction partners of oligomeric A β , we used protein arrays with 8163 recombinant human proteins. We identified 324 proteins as potential interactors of oligomeric A β .

Based on the protein sequences identified in the above mentioned experiments we wanted to extract such peptide subsequences that could inhibit binding of A β to these proteins. Such peptides could be a base set in the design of new, putative neuroprotective compounds. Using a mathematical algorithm we devised a peptide chip containing 4000 hexapeptides with sequences from the previously identified proteins and performed a binding experiment with oligomeric A β (1-42). We have demonstrated interaction of several peptides with A β . Some of these peptide sequences were synthesized and those of them which showed inhibitory effect on the toxicity of A β in MTT test were used further experiments. We will use these peptides as lead compounds in rational drug design against AD.

Acknowledgement

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ELEMENTAL ANALYSIS OF PROTEINS BY ION BEAM BOMBARDMENT

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Abstract

Identification, quantification and location of metal ions bound to proteins and enzymes are very essential experimental steps in biochemistry, enzymology and related sciences on the way to understand the structure and function of these biological macromolecules and the role played by the particular metal of interest. In addition to the most commonly used chemical and biochemical analytical methods the novel nuclear technique called ion beam analysis (IBA) could also be very effective and sensitive for these purposes in certain cases. The basic idea of an IBA technique is very simple. Bombarding a sample by a beam of ions accelerated to few MeV energy by a particle accelerator several atomic and nuclear processes take place (elastic scattering of the bombarding particles (BS), ionisation inner atomic shells of the target atoms and the subsequent production of characteristic X-rays (PIXE), isotope sensitive nuclear reactions mainly on lighter elements including C, N and O (ANR) etc.. The determination of N might have special importance in studying biological macromolecules, because nitrogen content can be used to quantify the total protein content of the analysed volume. In the field of life sciences PIXE is the most frequently and successfully used technique offering simultaneous detection of elements ranging from Al to U with sensitivities in the ppm range under usual experimental conditions. The amounts (or concentrations) of the detected elements can be calculated from the area under the well separated. Precise and accurate bulk trace element concentrations are certainly very important but the basic questions to be answered are usually the followings. What kind of metal ion is bound to the particular metalloprotein of interest and what is the number of those ions in a protein molecule? To answer such structure (and consequently also function) specific questions about the binding sites of the ions, the simple elemental analysis of the whole protein molecule is not sufficient alone. Dedicated cleavage of the composite macromolecule, careful separation of the well characterised subunits obtained, and keeping track of metal ions by subsequent elemental analysis could be a method to apply: the ion beam technique should be combined with suitable biochemical separation process. Direct PIXE scanning of polyacrylamide gel electrophoretograms (the PIXE-PAGE method) proved to be a unique way to locate metal-containing bands, identify and even quantify to a certain extent the metal ions in them [1]. In cellulose acetate electrophoretograms the simultaneous N determination is also possible.

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L-15
**MOLECULAR APPROACHES FOR THE INVESTIGATION OF MASS
TRANSFER PHENOMENA IN CHROMATOGRAPHY**

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Abstract

The study of the details of mass transfer in liquid chromatography is of central interest. We apply the microscopic (or molecular dynamic) model of chromatography to study the reversed phase separation of small and large molecules. The microscopic theory of chromatography describes the evolution of a chromatographic peak as the random migration of the molecules along the column combined with adsorption–desorption processes that occur at random, too.

The molecular dynamic model is rather straightforward to comprehend and it can furnish direct answers when one tries to understand the development of chromatographic peaks. We show that the microscopic model can be rather simply used to estimate the fundamental characteristics of the separation process. We can estimate the rate a molecule is adsorbed on the surface of the stationary phase while it migrates along the column.

When combining the general rate model with the molecular dynamic model, one can consider and compare the kinetics of the transfer of solute molecules between the flowing and stagnant zones of mobile phase, the pore diffusion, etc.

We analyze the peak shapes recorded under linear conditions, and can characterize the heterogeneity of the surface of the stationary phase. With a peak shape analysis that is based on the molecular dynamic model of chromatography, we can identify the presence of heterogeneous mass transfer or adsorption kinetics. We can, furthermore calculate the amount of retention due to the individual adsorption sites.

The general rate model of chromatography, which is a macroscopic model, offers the most detailed description of the separation process. We compare the results provided by both microscopic and macroscopic analysis of the peak shapes and statistical moments.

In this paper we discuss the influence of wide pore-size distributions. We present results obtained on nonporous, fully porous, and fused-core particles. Furthermore, mass transfer in supercritical fluid chromatography and reversed-phase liquid chromatography are compared.

L-16

NEW INSIGHTS INTO THE RETENTION MECHANISMS ON STRAIGHT-CHAIN PERFLUORINATED STATIONARY PHASES FOR HPLC

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Abstract

Perfluorinated alkyl adsorbents are in the midst of renewed interest in several branches of the chemical-physical sciences, including proteomics, metabolomics, chiral resolution, recycling and reuse of catalysts, environmental sciences. In all of these applications, essentially, the concept fluorophilicity, that is the extraordinary capability exhibited by substrates with perfluoroalkyl moieties of selectively interacting, is exploited.

The retention mechanisms of a series of n-alkylbenzene homologues and several perfluoroalkyl acids have been studied on perfluorinated materials prepared with different bonding densities. Several features of these materials, including their adsorption properties from acetonitrile-water mixtures, their geometric characteristics and wetting properties, the effect of the bonding density on retention and selectivity (both methylene- and perfluoromethylene-selectivity) have been evaluated.

The information obtained by this study has allowed to interpret some particular aspects characterizing the chromatographic behavior of these phases, such as for instance the U-shape retention of perfluoroalkyl acids by changing the mobile phase composition, the poor chromatographic performance with highly aqueous mobile phases (water > 95% v/v) and their alternative selectivity with respect to traditional C18 adsorbents.

L-17

DESIGNING AND PREPARATION OF MULTIPLE CHROMATOGRAPHIC PACKINGS IN MICROCHIP

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Abstract

The dream of the lab-on-a-chip conception is to miniaturize a complete chemical laboratory into a microchip format. Since currently the most widely used separation technique in the analytical laboratories is the liquid chromatography (LC), surprisingly only relatively few chip-based chromatographic systems [1-3]. compared to chip-based capillary electrophoretic devices are known.

Here we report on a simple method to fabricate microfluidic chip incorporating multi-channel systems packed by conventional chromatographic particles without the use of frits [4]. The retaining effectivities of different bottlenecks created in the channels were studied. For the parallel multi-channel chromatographic separations several channel patterns were designed. The obtained multipackings were applied for parallel separations of dyes. The implementation of several chromatographic separation units in microscopic size makes possible faster and high throughput separations.

The simplicity of the replication of the polydimethylsiloxan (PDMS) chips and the minimal consumption of the conventional packing particles (some tens of nanograms for a 10 mm length of packing) makes the chips inexpensive and disposable.

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L-18

FAST AND RELIABLE URINE ANALYSIS USING A PORTABLE PLATFORM BASED ON MICROFLUIDIC ELECTROPHORESIS CHIPS WITH ELECTROCHEMICAL DETECTION

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Abstract

A novel ready-to-use portable microfluidic platform was adapted for analysis of uric acid and related compounds in urine samples. Microfluidic devices, especially microchips electrophoresis (ME), are very attractive for clinical and pharmaceutical analysis. Thus, a novel portable and easy-to-handle instrument, HVStat (165 x150 x85 mm), based on microfluidic electrophoresis chips with amperometric detection was used for the determination of uric acid and interfering compounds (ascorbic acid, paracetamol, epinephrine.) in urine samples. Moreover, the microfluidic platform performance is controlled by a user-friendly PC interface (MicruX Manager) especially designed for the use of microchips electrophoresis with electrochemical detection. The adapted analysis methodology at portable microfluidic platform allows the separation and detection of uric acid and related compounds in less than 90s with minimal sample pre-treatment. Thus, the uric acid is directly detected without previous enzymatic based-reactions or other complex pretreatment. The urine sample is simply diluted in the buffer solution and injected directly in the microchip where the uric acid is separated and detected at platinum electrode of a SU-8/Pyrex microfluidic chip. The microfluidic chips were used for several analyses with a good performance and precision, decreasing drastically the cost and time per analysis.

Thus, the complete microfluidic platform, including the main instrument, reusable holder and microchips, has been demonstrated as an excellent analytical tool for fast and reliable urine analysis.

This work has been supported by the Spanish Ministry of Science and Innovation (MICINN – PTQ-09-01-00263, PTQ-09-01-00264 and PTQ-10-02730) and Principality of Asturias (FICYT – IE09-281)

L-19

OPEN CHIP SAW-MALDI MS SAMPLE HANDLING

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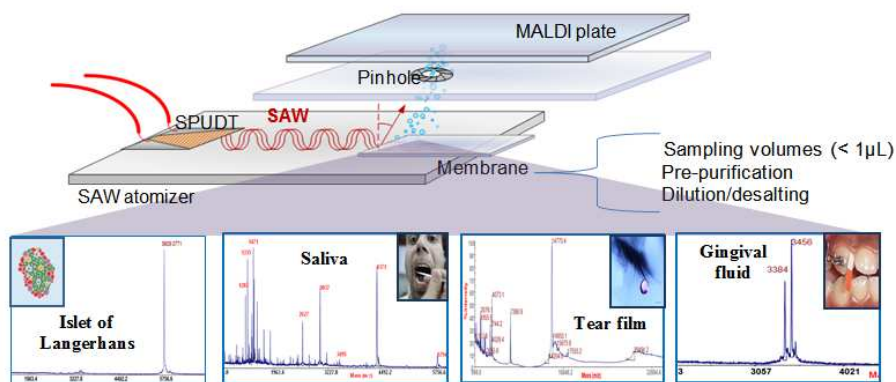
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Abstract

SAW atomizer has been interfaced with MALDI MS for fast analysis of small volumes (< 1µL) sampled in a membrane¹. SAW propagate through and underneath the membrane and atomize the liquid bound sample into 2-10 µm diameter aerosol which is subsequently deposited on a MALDI plate for further analysis². Fast peptide profiling of living islets of Langerhans and bio fluid (saliva, tear film) has been achieved and an adaptation for the analysis of living agarose-entrapped cancer cells is currently under development. MALDI MS of a single beta cells and a single islet using the acoustic levitation technique³ leads to a wall less analysis with low contamination and high sensitivity⁴.



Preliminary results, together with a representation of the basic SAW-MALDI sample preparation method.

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Abstracts

Posters

P-01

EXPERIMENTAL VALIDATION OF THE MOLECULAR THEORY OF SIZE-EXCLUSION CHROMATOGRAPHY WITH WIDE PORE SIZE DISTRIBUTION

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Abstract

The stochastic model of size-exclusion chromatography (SEC) using the characteristic function was developed by Dondi et al [1]. The model allows taking into account the kinetics of the pore ingress and egress processes, the heterogeneity of the pore size and polymer polydispersion.

The stochastic model of SEC describes the chromatographic process as random process in which molecules undergo a continuous exchange between the moving interstitial zone and the stagnant zone inside the pores of particles. The retention of the macromolecules rises from the hydrodynamic chromatography effect and the size-exclusion effect. The retention of the excluded samples comes from only the hydrodynamic chromatography effect.

A new chemometric procedure was presented by Pasti et al. [2] for the estimation of equilibrium distribution constant of size-exclusion effect (K_{SEC}). $K_{SEC} = (1 - \rho)^m$

where ρ is the macromolecule size relative to pore size, m is the total size factor exponent which depends on the pore shape. When m is equal to 1, 2 or 3, the pores are slit shaped, long cylindrical or conical [3].

In this study we will show, how to estimate the pore volume, the pore size, and the pore size distribution of particles on the basis of experimental data using a chromatographic model extended to wide pore size distribution in case of cylindrical and conical pore shape in core-shell particles.

The work was supported by the grants TÁMOP-4.2.1. B-10/2/KONV-2010-0002, TÁMOP-4.2.2.A-11/1/KONV-2012-0065, and OTKA K 106044.

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P-02

APPLICATION OF CAVITAND DERIVATIVES ON HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

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Abstract

Cavitands are cavity-shaped cyclic oligomers and they can create host-guest interactions with various analytes. Host-guest interaction represents the affinity of macrocyclic molecules to form reversible complexes with neutral as well as charged molecules.

Cavitands (e.g.: calixarenes, resorcinarenes, cyclodextrins and their derivatives) may have three types of uses in liquid chromatography. Stationary phases can be synthesized by covalently bonding cavitands on silica particles. Many cavitand-bonded silica phases are prepared for the separation of aromatic positional isomers [1, 2], enantiomers of chiral compounds [1] and polycyclic aromatic hydrocarbons [2]. Furthermore, cavitand derivatives can be applied as mobile phase additives [3]. Cavitands are also employed as dynamic coatings on RPLC stationary phase for the separation of aromatic positional isomers and nucleobases [4].

We investigated chromatographic behavior and possibilities of the use of resorcinarene derivatives in high performance liquid chromatography.

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P-03

FABRICATION OF MICROCHIPS WITH MULTICHANNEL SYSTEMS

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Abstract

Different microfluidic systems with connected or independent multiple channels were developed. In the channels of these microchips several parallel chromatographic packings can be created.

A new packing procedure was developed, a bottleneck was created in a channel of 100 micron width, and around 1 microliter of suspension of methanolic C18 particles was injected into the chip channel toward the bottleneck and then washed with methanol [1]. The particles retained around the bottleneck, and then the newly arrived particles adhered to the packing; increasing its length. The first particles acted as keystones blocking the other particles [2].

Two different procedures were developed to create the bottleneck in the channels. In the first case the bottleneck was the result of a line in the photolithographic mask. In the other case an 8-10 micrometer wide and 50 micrometer long channel was drawn into the photolithographic mask as a bottleneck. Both procedure was suitable for the making of chromatographic packings in parallel channels. The second procedure was used to integrate the chromatographic packings into the channels because it was more reproducible bottleneck fabrication procedure.

One of the great advantage of these systems is the possibility of making parallel measurements at the same time.

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P-04

DETERMINATION OF TEMOZOLOMIDE IN SERUM AND BRAIN TUMOR WITH MICELLAR ELECTROKINETIC CAPILLARY CHROMATOGRAPHY

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Abstract

Temozolomide (TMZ) is an anticancer drug and can be considered as the most frequently used alkylating agent for the treatment of malignant primary brain tumors (e.g. glioblastoma). The main problem regarding the chemotherapy against brain tumors is the low drug effectiveness due to the moderate penetration rate through the blood-brain barrier. The TMZ crosses the blood-brain barrier, but its exact local concentration in the human brain tumor tissue has not been determined.

Micellar electrokinetic capillary chromatography (MEKC) was applied to determine TMZ in human serum and brain tumor. In our earlier publication it was demonstrated that the MEKC is a useful technique to determine TMZ in model solution [1]. The TMZ could be detected in in vivo serum samples without sample pretreatment. The brain tumor tissues (0,3 g-0,8 g) were lyophilized and extracted with ethyl acetate to preconcentrate the analyte and obtain an injectable sample. The lyophilized tumor samples were dissolved in minimal volume (300-600 µl) of 0,1 M HCl. The obtained viscous solutions were centrifuged (9000g for 15 min). 50 µl supernatants have been extracted with 3 x 300 µl ethyl acetate (10 min vortex). After removing the organic solvent with rotary vacuum evaporator, the dried material was dissolved into 10 µl 0,1 M HCl, and was injected. The precision of migration times and peak area were 1,07 and 1,48 RSD% respectively. The limit of quantitation (LOQ) was 0,096 µg/ml using on capillary UV detection at 325 nm. The obtained peak concentration (8,2-10,1 µg/ml) and T_{max} (0,5-1,5 h) of TMZ in serum sample [2] were similar to the data reported by others [3], in vivo TMZ concentration found in brain tumor ranged between 0,046-0,117 µg/g.

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P-05
DETERMINATION OF THE OAT1, OAT3 AND BCRP SUBSTRATE
CHLOROTHIAZIDE BY LC-MS/MS

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Abstract

Chlorothiazide is used as diuretic to manage excess fluids associated with congestive heart failures, hepatic cirrhosis, and corticosteroid/estrogen therapy. Chlorothiazide has also been found useful in the management of edema and hypertension. However, chlorothiazide intake is associated with adverse effects such as renal failure, renal dysfunction and interstitial nephritis. The mechanism of action of chlorothiazide-mediated diuretic effect and associated side effects remain poorly understood. We hypothesize that chlorothiazide is actively uptaken by OAT1 and/or OAT3 and that this active uptake together with its BCRP-mediated efflux contributes to its rapid renal excretion.

Chlorothiazide levels in the transport assays carried out to examine the kinetics of OAT1- and OAT3-mediated chlorothiazide transport, as well as inhibition of chlorothiazide uptake by probenecid, furosemide, and diclofenac were determined with a simple LC-MS/MS method. The chromatographic separation was carried out on a Poroshell 120 EC-C18column. Mobile phases were 0.1% formic acid in water (A), and 0.1% formic acid in acetonitrile (B) with isocratic elution (B=20%) at a flow rate of 0.5 mL/min. The detection was performed on a triple quadrupole tandem mass spectrometer by MRM via electro spray ionization source with negative mode. The lower limit of quantification was 1 nM. Results were accepted following FDA's Guidance.

Chlorothiazide uptake was markedly higher into transfected cells compare to parental cells and the uptake could be inhibited by probenecid, diclofenac and furosemide in a dose dependent manner. In this study we showed that chlorothiazide is a substrate of OAT1, OAT3 and BCRP. These findings might explain the rapid renal secretion of chlorothiazide and might help understanding the molecular basis of the observed adverse effect of chlorothiazide.

P-06

IDENTIFICATION OF MPL-W515L MUTATION IN THROMBOPOIETIN RECEPTOR -COULD BE MPL-W515L MUTATION AN ADDITIONAL VASCULAR „RISK FACTOR” IN WOMAN DIAGNOSED WITH ESSENTIAL THROMBOCYTHEMIA?-

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Abstract

Background: Essential thrombocythemia (ET) is a clonal BCR-ABL1-negative myeloproliferative neoplasm (MPN). Life expectancy of ET patients is strongly affected by thrombotic events. Investigation of risk factors of thrombotic events in ET women should be important, since changes in their lifetime conditions such as pregnancy or climacterium could have an additional effect on the relatively frequent occurrence of vascular complications. 30–40% of ET patients are JAK2 V617F mutation negative, thus, further mutation analysis could be important. [1] Our aim was to evaluate the frequency of acquired MPL W515L mutation, in JAK2 V617F-negative ET woman patients and to answer the question whether the MPL-W515L mutation has an additional role as a vascular „risk factor” in ET women? **Patients and methods:** Between 1999 and 2011, 96 patients with essential thrombocythemia were selected randomly. Among them 27 JAK2 V617F-negative female ET patients could be found with the mean age of 55.5 years [range: 14–95]. DNA was isolated from EDTA stabilized peripheral blood samples, and screened for the mutation by allele-specific PCR reactions and subsequent agarose gel electrophoresis. The method has 1% to 5% sensitivity in terms of allele frequency. **Results:** The MPL W515L mutation could be detected in 16 patients. Mann-Whitney tests, and multivariate binary logistic regression was run to estimate the probability of thrombotic events in combination with MPL mutation status, and with other main cardiovascular risk factors. The MPL mutations - although not significantly due to the small sample - showed a correlation with the clinical appearance of the disease, and its possible prognostic value could be detected in our group of patients. **Conclusion:** Based on our findings we suppose that ET female patients with cardiovascular risk factors (especially high blood pressure, hyperlipidemia, smoking) may have a higher risk for thrombotic events, and the MPL-W515L mutation could have an additional role in this special group of patients.

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P-07

INFLUENCE OF CULTURE PARAMETERS ON PHENOL BIOSORPTION BY LYOPHILIZED MYCELIAL PELLETS OF *PHANEROCHAETE CHRYSOSPORIUM*

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Abstract

The biosorption of phenol from aqueous solution on non-living (treated with heat and pressure) lyophilized mycelial pellets of *Phanerochaete chrysosporium* cultivated in liquid medium having various composition was studied in a batch biosorption system. The fungal cell surfaces were characterized by FTIR spectroscopy and specific surface charge detection. The effect of pH, contact time, initial phenol concentration and biosorbent dosage on biosorption process was systematically studied for biosorbents. The maximum phenol uptake by various fungal preparations was observed at pH 5-6. Adsorption kinetics and isotherms were determined and evaluated at an initial pH of 5.5. For adsorption kinetic and equilibrium study by both bioadsorbents a comparative evaluation is presented using non-linear least-squares estimation and linearization of Langmuir and anti-Langmuir equations [1]. The presence of mineral and vitamin materials in the liquid medium enhanced the sorption capacity of fungal biomass for phenol. The mycelial pellets will be used as a column material for dynamic adsorption study.

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Acknowledgement

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P-08

DEVELOPMENT AND INVESTIGATION OF SUBCUTANEOUS HYDROGEN SULFIDE (H₂S) ABSORPTION USING MICRO BIOSENSOR

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Abstract

Hydrogen sulfide (H₂S) is a naturally occurring poisonous gas. Analysis of it in environmental or sewage samples has been an important task. H₂S gas can be found in 20 μmol/dm³ concentration in the tissues of living animals too. Recently the involvements of H₂S in numerous physiological processes have been proved. This generated a rapidly increasing interest in studying its interaction with enzymes, with hemoproteins. Its role as a signaling molecule of the inflammatory and nervous systems, and in cardiovascular system has been proved. It also regulates vascular tone. Today H₂S is considered as member of the group of physiological signaling gases together with the NO and CO.

New investigations are dealing with the role of H₂S in peripheral nervous system, in neuro degradation processes, in reactions in gastrointestinal and endocrine organs, as well as the impact of it in pain.

Some thermal waters used in balneotherapy have significant amount of dissolved H₂S that may have important role in treatments. For studying the extent of absorption, and local concentration changes appropriate measuring method and apparatus are needed.

The H₂S is a redox-sensitive unstable molecule, and its concentration is relatively small in the complex chemical composition of living tissues. Measuring its instantaneous local concentration is a difficult task. We introduce a sensor cell developed for sensitive amperometric H₂S detection in “*in vivo*” measurements. The dynamic concentration range, the lower limit of detection, the selectivity, stability of the cell were studied. Its applicability was proved detecting the absorption of H₂S through the skin of anesthetized mice test animals.

Acknowledgement

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BIODEGRADATION AND ADSORPTION PROPERTIES OF CANDIDA TROPICALIS CELLS IN AQUEOUS SOLUTIONS

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Abstract

In our present work we investigate a live microorganism culture, which can use phenol as carbon source in its metabolism, so it can biosorb and biodegrade this pollutant. *Candida tropicalis* was chosen for model culture. This yeast can live and grow at a relative high phenol concentration [1], so we can probably use it to remove phenol from polluted water. Lyophilized cells were used for phenol biosorption and biodegradation study in aqueous suspension. Lyophilized and inactivated (heat treated) cells were also investigated as possible adsorbent for phenol removal from aqueous solution. Less amount of phenol was removed by lyophilized and deactivated cells, than by lyophilized and active culture, but this deactivated biomaterial was more usable and showed reproducible results.

An inorganic pollutant was also studied in this work. We investigated the facility of using *Candida tropicalis* to remove copper(II) from aqueous solution. The next step in our work will be the competitive adsorption study of organic and inorganic pollutants by lyophilized cells and immobilization [2] for column and dynamic adsorption study.

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DEVELOPMENT AND APPLICATION OF LCMS AND LC-FLD METHODS FOR
THE ANALYSIS OF KYNURENIC ACID AND A NOVEL KYNURENIC ACID
ANALOG IN MOUSE SERUM

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Abstract

Kynurenic acid (KYNA) is a widely studied metabolite of tryptophan, formed through the kynurenine pathway. It is known to exert endogenous protection against the toxic effects of other kynurenine pathway metabolites, such as quinolinic acid and 3-hydroxy-L-kynurenine, and those of other excitotoxins. The possibility of its therapeutic use therefore emerges, including treatment of disorders of the central nervous system [1]. However, the chemical and pharmacokinetic properties of KYNA hamper its use in preclinical studies. In higher doses, its solubility is a limiting factor, it penetrates the blood-brain barrier poorly, and it undergoes a rapid clearance from the brain and the body, this clearance being mediated by organic anion transporters. To overcome these disadvantages and/or improve pharmacodynamic properties, numerous derivatives or prodrugs have been synthesized, including a novel KYNA amide [2].

The aim of the present study was to examine the serum pharmacokinetics of the synthesized KYNA amide. Special attention was paid to the possible metabolism of this analog to KYNA. For the determination of KYNA and a novel KYNA analog in mouse serum samples following a sample preparation procedure based on protein precipitation, new high-performance liquid chromatographic methods with fluorescence and mass spectrometric detection were developed. The analytical parameters obtained in the validation procedure suggest that the developed method with mass spectrometric detection is simple, fast, accurate and suitable for the measurement of KYNA and its analogs [3].

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P-11

ANALYZING GLUTAMATE AND ASPARTATE ENANTIOMERS IN BRAIN TISSUE SAMPLES BY CE-LIF

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Abstract

Aspartate and glutamate are the two major excitatory neurotransmitters in the CNS, playing central role in learning processes and memory formation. While the function of glutamate is well known, the role of aspartate is less well understood. It has been suggested, that its non-proteogenic *D*-enantiomer has an effect in the regulation of neurotransmission, neurogenesis and neuronal plasticity, as it occurs naturally in the CNS.

Due to its excellent separation efficiency capillary electrophoresis is perfectly suitable for enantiomer separation. Laser induced fluorescence (LIF) detection was chosen due to its better sensitivity compared to the conventional UV absorbance detection. Because of the lack of easily detectable moiety, prior to analysis sample derivatization providing a fluorophore group is needed.

In our work a capillary electrophoresis method has been elaborated in order to achieve chiral separation of fluorescently labeled aspartate and glutamate. A dual cyclodextrin system has been found to provide the appropriate chiral and chemical selectivity. Reverse polarity mode in coated capillary has been used to achieve acceptably short analysis time. The developed method has been validated and used for the analysis of brain tissue samples. *D*-Asp concentration has been found to be in the range of 20-30 nmol/g in the striatum of one day old domestic chickens. Higher concentration of *D*-, but not *L*-Asp has been measured in the subventricular proliferation zone, where the neurogenesis mainly takes place, compared to a non-proliferative control region (nidopallium). It has also been shown that the *D*-Asp / total aspartate concentration ratio decreased during the first 4 days of development. These results support a specific involvement of *D*-Asp in the neurogenesis of young domestic chicks.

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P-12

STRATEGY FOR IDENTIFICATION OF DISULFIDE BRIDGES IN A CYSTEINE RICH PROTEIN

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Abstract

Mass spectrometric methods for disulfide bridge identification are based on chemical and enzymatic methods (according to the sequence of protein or peptide), and produce a mixture of peptides containing only one disulfide bond. Fragments linked together through disulfide bridges are separated and analyzed by capillary reversed phase HPLC coupled to the mass spectrometer. The fragments can be identified based on their unique masses and tandem mass spectrometric fragments. The success of the procedure usually depends on the reagents used for cleaving the peptide or protein between the half cystinyl residues. Based on the sequence of PAF (antifungal protein), a mixture of trypsin and chymotrypsin was found to be a good choice for enzymatic cleavage. However, identification of the SS-pattern by enzymatic digestion followed by MS may be difficult because of the extreme stability of some disulfide proteins, especially PAF. This protein showed high enzyme resistance, that is, even after 12 h proteolytic digestion a significant amount of undigested peptide was found in the samples. Enzyme resistance can be the consequence of inaccessible cleavage sites. In our work the enzymatic method was compared with a chemical cleavage based on partial reduction of disulfide bridges with TCEP (tris(2-carboxyethyl)phosphine) followed by cyanilation (1-cyano-4-dimethylaminopyridinium tetrafluoroborate) under mild acidic conditions.

P-13

ZONE ELECTROPHORESIS ON MICROCHIP FOR BIOMOLECULES

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Abstract

Zone electrophoresis of the labeled amino acids on a commercially available lab-on-a-chip instrument was possible in a background electrolyte (BGE) without stabilizing detergents, which is in contrast to conventional CE; moreover, analysis times were drastically shorter than 10 s range. [1,2]

In our work we label amino acids (glycine, lysine, asparagine acid, glutamine acid) with two fluorescence dyes: fluorescein isothiocyanate (FITC) detected by the blue laser (λ_{ex} 450 nm) and cyanine 5 (Cy5) detected by the red laser (λ_{ex} 630 nm). FITC is a derivative of fluorescein which functionalized with an isothiocyanate reactive group (-N=C=S) to the original fluorescein to replace a hydrogen atom on the ring structure. FITC has excitation and emission spectrum peak wavelengths of approximately 495 nm/521 nm.

Cy5 dye belongs to the sulfoindocyanine dyes. The dye contains a short aliphatic side chains, which contains one or more highly reactive functional groups such as N-hydroxysuccinimide or maleimide. Cy5 dye excitation wavelength is 670 nm, while the absorption wavelength is 649 nm.

In our measurement we used modified DNA script. The running buffer was 100 mM sodium borate (pH 8.3). The amino acid samples were labeled for 24 hours at 4 °C.

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**RETENTION AND MASS-TRANSFER PROPERTIES OF INSULIN ON
SUPERFICIALLY POROUS AND TOTALLY POROUS REVERSED PHASES IN
HPLC**

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Abstract

Separation techniques have undergone considerable developments in the second half of the last century. The development of the chromatographic instrumentation was necessary in parallel with the development of stationary phases (of special packing materials) and columns. The developments and the availability of high-performance instrumentation and high-quality stationary phases have substantially supported the growth of HPLC researches and applications. In addition, new and also special instrumentation and columns for RPLC are continuously developed and marketed today. The stationary phases are the 'heart' of the chromatographic separations.

The RP-HPLC retention mechanism is still an important research area. Today, researchers seek a better understanding of processes of retention and selectivity. The interpretation of these processes at the molecular level, as well as their connection with the physical-chemical properties of the stationary phases is particularly important. There are different theories to envision the retention mechanism in reversed-phase chromatography (RP-HPLC). The most important ones are the well known hydrophobic interaction theory, the theory of partition and the adsorption theory.

In our work we aim to test and compare the different types (porous and superficially porous) of reversed phase packing materials; taking into account both the bioactive low-molecular-weight compounds and high-speed HPLC separations, as well as the determination of mass-transfer coefficients.

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**SCREENING OF USED WOODEN RAILWAY SLEEPERS CHEMICAL
COMPOSITION BY MEANS OF GAS CHROMATOGRAPHY – MASS
SPECTROMETRY**

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Abstract

The protection of wooden railway sleepers from biodegradation by impregnating them with coal tar or creosote has proven to be effective for the long term. However coal tar or creosote contains toxic polycyclic aromatic hydrocarbons (PAH) at high concentrations. The investigation of recycling of used sleepers in large amounts has become of great interest [1]. The screening of PAH's in wooden railway sleepers used in Lithuania, was carried out. Sample preparation was based on cold extraction of the PAHs using organic solvent and their determination was carried out by GC-MS. In this study different wood conifer tree railway sleepers and oak tree sleepers were investigated. One of the tasks was to determine extraction solvent efficiency. Several organic solvents were tested – methanol, n-hexane, benzene. Preliminary studies show, that conifer tree railway sleepers contain more PAHs comparing with oak tree sleepers. Several PAHs were identified, namely naphthalene, acenaphthene, fluorene, anthracene, phenanthrene, fluoranthene, pyrene, crysene, benzo[c]phenanthrene. Quantitative and qualitative analysis results will be revealed in this presentation.

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P-16

STEREOSELECTIVE ANALYSIS OF AMINO ACIDS AND ENDORPHIN ANALOGUE TETRAPEPTIDES BY CAPILLARY ELECTROPHORESIS

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Abstract

Stereoselective separations of members of two amphoteric molecule families (dansylated amino acids (Dns-AA) with apolar or acidic side chains, endomorphin-1 and -2 and their biologically active diastereomeric tetrapeptide analogues [1]) have been accomplished by capillary electrophoresis applying β -cyclodextrin derivatives (BCD) as selectors. The measured isoelectric point values were between pH 3.5-3.8 for the Dns-AAs, and 8.3-8.9 for the tetrapeptides. Accordingly, two –recently developed- cationic CDs, namely the permethylated monoamino BCD and the randomly methylated monoamino BCD and their neutral analogues (permethylated-BCD and randomly methylated BCD) were chosen as selectors for Dns-AAs. In case of the endomorphin analogues neutral CDs (permethylated-BCD and hydroxyl propylated BCD) or anionic ones (carboxymethylated-BCD or sulfobutyl ether BCD) were applied for the stereoselective analyses. In order to improve the resolutions the complex stability constants and the mobilities of the complexes were determined and in addition the pH and the CD concentrations were optimized. Reversals in enantiomer migration order were observed by varying pH or selector concentrations providing possibility to select the appropriate migration order for a given analytical problem. Consequently, good chiral separations of each investigated analyte could be carried out. Furthermore, mixtures of the Dns-AAs were successfully separated as a model of the real biological, environmental and food samples.

We gratefully acknowledge the Jedlik Ányos Grant (NKFP_A3-2008-0211 NATURSEP) for the financial support

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DETERMINATION OF SELECTED BACTERIAL PROTEINS FROM 2-D SDS-PAGE BY USING MALDI-TOF-MS**P. Pomastowski¹, B. Buszewski¹, K. Hrynkiewicz², M. Gawin³, W. Piekoszewski^{3,4}**¹*Department of Environmental Chemistry and Bioanalytics, Faculty of Chemistry, Nicolaus Copernicus University, Gagarina 7, 87-100 Toruń, Poland, email: bbusz@chem.uni.torun.pl*²*Department of Microbiology, Institute of General and Molecular Biology, Nicolaus Copernicus University, Lwowska 1, 87-100 Toruń, Poland, e-mail: hrynk@umk.pl*³*Laboratory of High Resolution Mass Spectrometry, Regional Laboratory of Physicochemical Analysis and Structural Research, Department of Chemistry, Jagiellonian University, ul. Ingardena 3, 30-060 Krakow, Poland, e-mail: gawin@chemia.uj.edu.pl*⁴*Toxicological and Pharmaceutical Analysis Group, Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University, ul. Ingardena 3, 30-060 Krakow, Poland, e-mail piekosze@chemia.uj.edu.pl***Abstract**

The study of bacterial proteome is based primarily on electrophoretic separation of a very complex protein mixture, via isoelectric point focusing and separation based on the protein mass. Proteomic studies typically include protein separation, identification, quantitative measurements, sequence analysis (bioinformatics), the study of the structure and finally the study of the interaction and modification of proteins. In recent years, two-dimensional gel electrophoresis (2-DE) has become the most widely used tool in proteomic analysis, because of its high resolving power for biopolymers complex mixtures. The essence of the research is a comparative analysis of protein expression, exposed to environmental factors and proteins in physiological state (undisturbed). A comparative analysis of the changes in protein expression, indicates a potential information about proteins that can be used in drug design and gives information about potential biomarker. Unique application of 2-DE provides broadening of possibilities in these fields. Furthermore, the technique of gel two-dimensional electrophoresis is undergoing an ascension, due to the possibility of coupling it with many analytical techniques. We describe an approach for mass spectrometric identification of proteins in proteome analysis via 2D-gel electrophoretic separation, using Coomassie Brilliant Blue staining procedures. The digested spots were analyzed by matrix-assisted laser desorption-ionisation mass spectrometry (MALDI-MS) [1-3].

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DETERMINATION OF MEAT ORIGINATED IMIDAZOLE DIPEPTIDES BY CZE

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Abstract

The imidazole dipeptides (carnosine and anserine) are widely distributed in vertebrate organisms and are particularly abundant in skeletal muscle and nervous tissue. Because of their physiological and therapeutic effects they can be considered as bioactive food components. These dipeptides as natural antioxidants in meat had significant importance also in point of the meat quality. It was developed a simple capillary zone electrophoretic method for separation of imidazole dipeptides. The CZE analysis was performed on a BioFocus 2000 system (BioRad) in uncoated fused-silica capillary total length 51 cm (45,5 cm effective length) and 50 μm I. D. The carrier electrolyte was 0.01-0.1 M phosphate buffer pH 2.5. The instrument was operating in thermostated temperature between 28 and 38 °C. The dipeptides were detected without derivatization at 200 nm. The optimum resolution of the examined compounds was found at 0.1 M buffer concentration and at the highest temperature. The analysis time was 12 minutes.

The method was used for analysis of raw meat samples and a number meat based food products, investigation of the release and resistance of carnosine in the gastrointestinal tract in an animal (rat) model.

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**MICROCHIP CAPILLARY ELECTROPHORESIS IN EXPRESSION PROFILING
OF CIRCULATING TUMOR CELLS FROM CANCER PATIENTS**

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Abstract

Capillary electrophoresis (CE) is a powerful, rapid, and effective bioanalytical method. The adaptation of capillary electrophoresis to microchips has made significant progress in enhancing the development of many CE applications. Microfluidic technology provides new ways to optimize sample handling procedures and DNA analysis for molecular diagnostics against cancer related markers. One example is the use of microchips in the detection of circulation tumor cells. The detection of circulating tumor cells depicts the dynamic process, whereas tumor cells located in bone marrow might be the result of a process that became static after the beginning of the illness.^[1] It is considered that the detection of the circulation tumor cells at an early stage offers a better chance to treat the cancer with higher effectiveness. Expression profiling of tumor markers associated to circulating tumor cells from cancer patients was evaluated using the DNA 1000 and high sensitivity DNA microchips. Prior to electrophoretic analysis the patients' blood samples had undergone immunomagnetic enrichment and multiplex RT-PCR. The high sensitivity DNA chip enabled detection of diagnostically valuable PCR fragments, which previously could not be detected by the DNA 1000 method, indicating its higher sensitivity and better diagnostic value.

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PHYTOCHEMICAL ANALYSIS AND CLASSIFICATION ACCORDING TO GROWTH SITES IN LITHUANIA OF *CHAMERION ANGUSTIFOLIUM* L. USING CHROMATOGRAPHIC AND RELATED TECHNIQUES

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Abstract

Chamerion angustifolium L. is one of the plants used for treatment of prostate cancer. Healing effect is addressed to certain flavonoids and tannins (mainly cyclic dimeric ellagitannin Oenothin B) [1] and some phenolic compounds which provide high antioxidant activity. *Chamerion angustifolium* L. was collected from different regional parts of Lithuania. Total amount of phenolic compounds, flavonoids and radical scavenging activity was determined spectrophotometrically and expressed in rutin equivalents (RE) mg/100 g. Highest total amount of phenolic compounds (14.446 and 14.005 RE mg/100g) and highest radical scavenging activity (17.442 and 17.347 RE mg/100g) was determined in 2SG and 6SG *Chamerion angustifolium* L. samples respectively. High Performance Liquid Chromatography – Diode Array Detector – Reaction Detector analysis technique was used to identify several phenolic acids in *Chamerion angustifolium* L. plant and determine individual peaks radical scavenging activities, where major peaks were identified as chlorogenic acid: 1SG and 3SG samples showed highest amounts (2685 RE mg/100 g ir 2527 RE mg/100g) respectively. The plant is known to accumulate very low amounts of volatile compounds. However, solid phase microextraction (SPME) preconcentration technique was used to preconcentrate headspace volatiles and GC-MS analysis revealed typical substances (cariophyllene, α -humulene, anethol, menthol, β -burbonene, β -ionone). These data were used to classify plants according their phytochemical differences. Different extracts of raw material were tested for phenolic and volatile compounds. Highest amount of volatile compounds was determined in 70% ethanolic extract where raw plant material was milled before maceration and extraction procedure. Minor amounts of β -burbonene, α -humulene, bicyclogermacene, α -bulnesene and linalool phenylacetate were determined in this extract.

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**INVESTIGATION OF TRANS-RESVERATROL AND STILBENE DERIVATIVE
TDPA IN HUNGARIAN WINES USING HPLC AND LC-MS**

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Abstrac

Plant polyphenols are naturally occurring secondary plant metabolites, synthesized in response to environmental stress factors. As being anti-oxidants and free-radical scavengers they serve as essential components of the human diet. Among polyphenols well studied representatives is the *trans*-resveratrol. *Trans*-resveratrol has been shown to modulate the metabolism of lipids, inhibit the oxidation of low density lipoproteins, reduce platelet aggregation is known to have anti-inflammatory, and has anti-tumor, cardio- and vasoprotective effects which plays a crucial role in the prevention of chronic cardiovascular and tumorous diseases.

In the present study, we investigate *trans*-resveratrol and the oxidative derivative of *trans*-resveratrol with a triple bond at the centre of the molecule: 3,4,5-trihydroxy-diphenylacetylene (TDPA) contain in wines. TDPA was first discovered by our research group. Twelve Hungarian wines were analyzed using HPLC/DAD and MS detection. The wines were from Villány wine region representing different wineries from 2008 to 2010 vintage years.

Our results show that *trans*-resveratrol and 3,4,5-trihydroxy-diphenylacetylene content is mainly dependent on variety and vintage year.

NHPLC-MS DETERMINATION OF DA AND DA METABOLITES IN MOUSE BRAIN

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Abstract

Background: Dopamine (DA) as an important monoaminergic type neurotransmitter plays an extremely important role in the central nervous system (CNS). The pathways of this neurosystem are divided to mesolimbic, mesocortical, nigrostriatal, medular-paraventricular, tuberoinfundibular parts and ultrashort DA cells. Through these pathways the coordination of movement, emotional reactions, motivation, food palatability, prolactin release are regulated, but DA is implicated in the control of nausea and vomiting as well. Among others Parkinson's disease, schizophrenia, hyperprolactinaemia are those pathological states, where overproduction or a decreased level of these molecules can be detected. The aim of our study is the quantitative analysis of DA and the metabolites of DA foundable in different brain regions.

Methods: Wet tissue samples were homogenised with acetonitril/water/trifluoroacetic acid solution, than ultrasonicated and filtered with CFD (Centrifugal Filter Device). The analysis was carried out by two instrumental systems, an Ultimate 3000 microHPLC-HCT ESI Ion Trap system. MRM (Multiple Reaction Monitoring) was used for the fragmentation. Maxis 4G UHR-QTOF MS was in ISCID (In-Source Collision-Induced Dissociation) fragmentation mode, an ion funnel was applied. The two instruments were coupled to the same HPLC system. DA and 3-methoxy-4-hydroxyphenethylamine (3-MT) were detected in positive, homovanillic acid (HVA) and 3,4-dihydroxyphenylacetic acid (DOPAC) in the negative ion mode.

Results: Using ESI Ion Trap system in MRM fragmentation mode DA levels show a significant difference in the nucleus acumbens. In the prefrontal cortex (PFC) just a trend ($p=0.11$) of DA concentrations could be sensed, but there was a significant difference among DOPAC levels.

Conclusions: Comparing the robustness and sensitivity of the two methods we decided to measure with the ESI Ion Trap on the basis of the better performance. Maxis QTOF system provides very high selectivity and sensitivity, but in ISCID fragmentation mode it shows lower sensitivity than ESI Ion Trap in MRM mode.

THIN METAL FILMS IN RESISTIVITY-BASED CHEMICAL SENSING

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The chemiresistor is the sensor, which changes its resistivity with change of adjacent chemical environment ^[1,2]. In this case it is the gold thin film sensor ^[3] interacting with thiols in liquid phase. When thiolated molecule adsorb on the gold surface and building self-assembled monolayer ^[4,5], there is established the covalent bond between the sulphur and gold atom with 50% of C-C bond strength ^[6]. Covalently bonded gold atoms do not participate on electric conduction anymore, thus gaining the resistivity of the layer. When the gold layer is sufficiently thin (<80nm), this effect become evident and the difference between clear and completely saturated surface can be represented by shift in resistance up to 5%. The device self was constructed as a microfluidic apparatus with four sensing elements arranged in the Wheatstone bridge to exclude influence of the temperature coefficient of resistivity. In ideal case, when the bridge is balanced, the voltage between the sensing nodes is zero. Only one element was used at a time. Sample was fed into the channels by quartz capillaries. The chip consists of two parts – glass plate with sensors and PDMS part with channels bonded together with aid of plasma activation. We tested dynamic range of the device by aliquote series of thiolated and non-thiolated compounds. The thiolated compounds were chosen the glutathione and cysteine, the non-thiolated were used tripeptide Gly-Pro-Glu and β -alanine because of their similarity to their thiolated counterparts.

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Pécs, the city of culture

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Pécs is the fifth largest city of Hungary, located on the slopes of the Mecsek mountains in the south-west of the country, close to its border with Croatia. It is the administrative and economical centre of Baranya county. Pécs is also the seat of the Roman Catholic Diocese of Pécs.

The city Sopianae was founded by Romans at the beginning of the 2nd century, in an area peopled by Celts and Pannoni tribes. By the 4th century it became the capital of Valeria province and a significant early Christian center. The early Christian necropolis is from this era which became an UNESCO World Heritage Site in December 2000.

Its episcopate was founded in 1009 by Steven I, and the first university in Hungary was founded in Pécs in 1367 by Louis I the Great. (The largest university still resides in Pécs with about 34,000 students). Pécs was formed into one of the cultural and arts center of the country by bishop Janus Pannonius, the great, Hungarian, humanist poet. Pécs has a rich heritage from the age of a 150 year long Ottoman occupation, like the mosque of Pasha Qasim the Victorious on Széchenyi square.

Name

The earliest name for the territory was its Roman name of Sopianæ. The name possibly comes from the plural of the Celtic sop meaning "marsh". Contrary to the popular belief, the name did not signify a single city and there are no traces of an encircling wall from the early Roman era, only from the 4th century.

The medieval city was first mentioned in 871 under the name *Quinque Basilicae* ("five cathedrals".) The name refers to the fact that when constructing the churches of the city, the builders used material from five old Christian chapels. In later Latin documents the city was mentioned as *Quinque Ecclesiae* ("five churches", a name identical in meaning to the German name *Fünfkirchen* and the Slovak name *Pät'kostolie*.

The name Pécs appears in documents in 1235 in the word *Pechyut* (with modern spelling: *pécsi út*, means "road to/from Pécs"). In Turkish "beş" means 5. The name is first recorded after the Mongol invasion of Europe. In other languages: in Latin *Quinque Ecclesiae*, in Croatian *Pečuh*, in Serbian *Печуј / Pečuj*, in Slovak *Pät'kostolie*, in German *Fünfkirchen*.

History

Ancient roman city

The area has been inhabited since ancient times, with the oldest archaeological findings being 6000 years old. Before the Roman era the place was inhabited by Celts. When Western Hungary was a province of the Roman Empire (named

Pannonia), the Romans founded several wine-producing colonies under the collective name of Sopianae where Pécs now stands, in the early 2nd century.

The centre of Sopianae was where the Postal Palace now stands. Some parts of the Roman aqueduct are still visible. When Pannonia province was divided into four administrative divisions, Sopianae was the capital of the division named Valeria.

In the first half of the 4th century Sopianae became an important Christian city. The first Christian cemeteries, dating back to this age, are inscribed on the World Heritage List. By the end of the century Roman rule weakened in the area, mostly due to attacks by Barbarians and Huns.

Early medieval city

When Charlemagne arrived in the area, it was ruled by Avars. Charlemagne, after conquering the area, annexed it to the Holy Roman Empire. It belonged to the Diocese of Salzburg.

A document written in Salzburg in 871 is the first document mentioning the early medieval city under the name *Quinque Basilicae*. During the 9th century the city was inhabited by Slavic and Avar peoples and was part of the Balaton Principality, a Frankish vassal state.

In the Middle Ages

According to György Györffy's theory from place names, after the Hungarians conquered the Carpathian Basin, they retained a semi-nomadic lifestyle changing pastures between winter and summer and Árpád's winter quarters -clearly after his occupation of Pannonia in 900- were perhaps in Pécs. Later, Comitatus of Baranya was established, the capital of the comitatus was not Pécs but a nearby castle, Baranyavár ("Baranya Castle".) Pécs, however, became an important religious centre and episcopal seat. In Latin documents the city was mentioned as *Quinque Ecclesiae*. Around 1000, the area was inhabited by the Black Magyars. The Deed of Foundation of the Diocese of Pécs was issued in 1009.

In 1064 when King Solomon made peace with his cousin, the later King Géza I, they celebrated Easter in Pécs. Shortly after the cathedral burnt down. The cathedral that stands today was built after this, in the 11th century.

Several religious orders settled down in Pécs. The Benedictine order was the first in 1076. In 1181 there was already a hospital in the city. The first Dominican monastery of the country was built in Pécs in 1238.

King Louis the Great founded a university in Pécs in 1367 following the advice of William, the bishop of Pécs, who was also the king's chancellor. It was the first university in Hungary. The founding document is almost word for word identical with that of the University of Vienna, stating that the university has the right to teach all arts and sciences, with the exception of theology.

In 1459 Janus Pannonius, the most important medieval poet of Hungary became the bishop of Pécs. He strengthened the cultural importance of Pécs.

Under Ottoman rule

After the Battle of Mohács (1526) in which the invading Ottoman army defeated the armies of King Louis II, the armies of Suleiman occupied Pécs. Not only was a large part of the country occupied by Ottomans, the public opinion of who should be the king of Hungary was divided, too. One party supported Ferdinand of Habsburg, the other party crowned John Zápolya in Székesfehérvár. The citizens of Pécs supported Emperor Ferdinand, but the rest of Baranya county supported King John. In the summer of 1527 Ferdinand defeated the armies of Szapolyai and was crowned king on November 3. Ferdinand favoured the city because of their support, and exempted Pécs from paying taxes. Pécs was rebuilt and fortified.

In 1529 the Ottomans captured Pécs again, and went on a campaign against Vienna. The Ottomans made Pécs to accept King John (who was allied with them) as their ruler. John died in 1540. In 1541 the Ottomans occupied the castle of Buda, and ordered Isabella, the widow of John to give Pécs to them, since the city was of strategic importance. The citizens of Pécs defended the city against the Ottomans, and swore loyalty to Ferdinand. The emperor helped the city and defended it from further Ottoman attacks, but his advisers persuaded him into focusing more on the cities of Székesfehérvár and Esztergom instead of Pécs. Pécs was preparing for the siege, but a day before, Flemish and Walloon mercenaries fled from the city, and raided the nearby lands. The next day in June 1543 the Bishop himself went to the Ottomans with the keys of the city.

After occupying the city the Ottomans fortified it and turned it into a real Ottoman city. The Christian churches were turned into mosques; Turkish baths and minarets were built, Qur'an schools were founded, there was a bazaar in place of the market. For a hundred years the city was an island of peace in a land of war. She was a sanjak centre in Budin Eyalet at first and Kanije Eyalet later as "Peçuy".

In 1664 Croat nobleman Nicholas Zrínyi arrived in Pécs, with his army. Since the city was well into the Ottoman territories, they knew that even if they occupy it, they could not keep it for long, so they planned only to pillage it. They ravaged and burned the city but could not occupy the castle. Mediaeval Pécs was destroyed forever, except the wall encircling the historical city, a single bastion (Barbakán), the network of tunnels and catacombs beneath the city, parts of which are closed down, other parts are in possession of the famous Litke champagne factory, and can be visited today. [citation needed] Several Turkish artifacts also survived, namely three mosques, two minarets, remnants of a bath over the ancient Christian tombs near the cathedral, and several houses, one even with a stone cannonball embedded in the wall.

After the castle of Buda was wrested from Ottoman rule in 1686, the armies went to capture the rest of Pécs. The advance guards could break into the city and pillaged it. The Ottomans saw that they could not hold the city, and burnt it, and withdrew into the castle. The army led by Louis of Baden occupied the city on

October 14, and destroyed the aqueduct leading to the castle. The Ottomans had no other choice but to surrender, which they did on October 22.

The city was under martial law under the command of Karl von Thüngen. The Viennese court wanted to destroy the city first, but later they decided to keep it to counterbalance the importance of Szigetvár, which was still under Ottoman rule. Slowly the city started to prosper again, but in the 1690s two plague epidemics claimed many lives. In 1688 German settlers arrived. Only about one quarter of the city's population was Hungarian, the others were Germans or Southern Slavs. According to 1698 data, South Slavs comprised more than a half of the population of the town. Because Hungarians were only a minority of the population, Pécs did not support the revolution against Habsburg rule led by Francis II Rákóczi, and his armies pillaged the city in 1704.

In modern times

A more peaceful era started after 1710. Industry, trade and viticulture prospered, manufactures were founded, a new city hall was built. The feudal lord of the city was the Bishop of Pécs, but the city wanted to free itself from episcopal control. Bishop George Klimó, an enlightened man (who founded the first public library of the country) would have agreed to cede his rights to the city, but the Holy See forbade him to do so. When Klimó died in 1777, Queen Maria Theresa quickly elevated Pécs to free royal town status before the new bishop was elected. This cost the city 83,315 forints.

According to the first census (held in 1787 by the order of Joseph II) there were 1474 houses and 1834 families in Pécs, a total of 8853 residents, of which 133 were priests and 117 were noblemen.

In 1785 the Academy of Győr was moved to Pécs. This academy eventually evolved into a law school. The first stonework theatre of the city was built in 1839.

The industry developed a lot in the second half of the 19th century. By 1848 there were 1739 industrial workers. Some of the manufactures were nationally famous. The iron and paper factories were among the most modern ones of the age. Coal mining was relevant. A sugar factory and beer manufactures were built, too. The city had 14,616 residents.

During the revolution in 1848–49 Pécs was occupied by Croatian armies for a short time, but it was freed from them by Habsburg armies in January 1849.

After the Austro-Hungarian Compromise of 1867 Pécs developed, like all the other cities and towns of the country. From 1867 Pécs is connected to the nearby town Barcs by railway, and since 1882 it is also connected to Budapest. In 1913 a tram system has been founded, but it was extinguished in 1960.

At the end of World War I Baranya county was occupied by Serbian troops, and it was not until August 1921 that Pécs could be sure that it remains part of Hungary. The University of Pressburg (modern-day Bratislava, Slovakia) was moved to Pécs after Hungary lost Pressburg according to the Treaty of Trianon.

During World War II Pécs suffered only minor damages, even though a large tank-battle took place 20–25 km south of the city, close to the Villány area late in the war, when the advancing Red Army fought its way towards Austria.

After the war development became fast again, and the city grew, absorbing several nearby towns. In the 1980s Pécs already had 180,000 inhabitants.

After the end of Socialist era (1989–1990) Pécs and its county, like many other areas, were hit hard by the changes, the unemployment rate was high, the mines and several factories were closed, and the war in neighboring Yugoslavia in the 1990s affected the tourism.

Pécs was also the centre of the Nordic Support Group (NSG) consisting of units from Denmark, Norway, Sweden, Finland and Poland, as part of the IFOR and later SFOR NATO deployments, after the Dayton Agreement and following peace in former Yugoslavia; the first units were deployed to Pécs in late 1995 and early 1996. The NSG handled the relaying of supply, personnel and other logistical tasks between the participating countries and their deployed forces in Bosnia-Herzegovina.

Pécs always was a multicultural city where many cultural layers are encrusted melting different values of the history of two thousand years. Hungarians, Croats and Swabians still live in peace together in economic and cultural polarity. In 1998 Pécs was given the UNESCO prize Cities for peace for maintaining the cultures of the minorities, and also for its tolerant and helping attitude toward refugees of the Balkan Wars. In 2007 Pécs was third, in 2008 it was second Liveable city (The LivCom Awards) in the category of cities between 75-200 thousand inhabitants.

In 2010 Pécs was selected to be the European Capital of Culture sharing the title together with Essen and Istanbul. The city's motto was: "The Borderless City". After receiving the title major renewal started in the city. Renewed public places, streets, squares and neighbourhoods, a concert hall, a new library and center and a cultural quarter were designed.

Attractions

UNESCO World Heritage

Cella Septichora Visitor Centre



The Centre introduces the most beautiful edifices of the 4th century Early Christian Burial Ground, which, owing to its unique value became part of the UNESCO World Heritage in 2000.

Cella Septichora

The largest building of the burial ground discovered so far. It was named after its septifoil layout (having seven apses) that is unique among

the Early Christian buildings.

Peter and Paul Burial Chamber

This 4th century building is located in the centre of the burial ground. We can admire the richly painted walls and the barrel vault of the burial chamber.

The Wine Pitcher Burial Chamber

This Early Christian burial chamber is located in a north-south direction including a grave with a double shell casing. Its name comes from the painted decoration (fresco) found in the recess of its northern wall.

The Octagon Burial Chamber

According to the most recent researches this chapel was possibly built to house the grave of a martyr. This much larger than usual building is not an isolated burial chamber but might probably have been a place of pilgrimage, a building partly sunk into the ground with windows.

Early Christian Mausoleum

As a result of the excavations of 1975-76, the biggest and most important Early Christian edifice, Mausoleum was unearthed in the descending space in front of the Cathedral.

The upper part of the double-storied building had been a chapel which was perished completely, and the lower level was a burial chamber that could be accessed through a stairway from the vestibule.



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The walls of the burial chamber are covered with frescoes of Biblical scenes. The fragmented though clearly visible paintings were applied on wet lime-cast with the fresco technique. A part of the mural series of the northern wall depicts the Fall of Adam and Eve with the serpent on the tree turning to Eve. The other painting shows Daniel in the Lions' Den. Next to Daniel banderoles can be seen starting from wreaths. Both scenes are framed by red stripes in a square. A Chi-Rho symbol, Christ's initials are painted above the round-arched niche in the eastern wall of the chamber. A painting on the left side of the niche can be seen only in fragments; possibly it depicts the enthroned Christ. The archment was also decorated with paintings. The lid of the marble sarcophagus is adorned with masked heads, and each side of it is decorated with a winged cherub.

The paintings and the sarcophagus in the World Heritage Mausoleum have been restored with the most up-to-date techniques, and their protection is ensured by a protective building above them. The reconstructed base of the former chapel can be seen above the burial chamber.

Sepulchral Structures of Apáca Street



A part of the extensive Roman burial ground located beneath the Cathedral Square was discovered here in 1958 when a construction was carried out in the yard of the library. First, a double grave with painted walls was found. This was built of brick and stone and covered with a pitched roof also made of brick. The inside of the grave was also painted.

A burial chamber with no paintings and several simple graves were also discovered nearby that had only some funerary goods. In the southern part of the yard a large collective tomb (crypt) was found with 14 graves. These were also covered with brick, the cover being stuck to the wall of the crypt with the help of lime mortar.

Researches date the remains back to the 4th century. When the Romans left, during the time of the mass migration of peoples, the graves were ravaged. The few that remained intact contain bracelets and beads, earrings and rings as well as glass vessels.

Of the graves in this part of the burial ground the double grave and its painted walls offer great experience. The decoration of the walls divided into three parts, the simple line drawing symbolize a gate with a circular pattern in the centre. On the gable of one of the graves we can see the Greek initials of the name of Christ (XP), the so called Christogram.

Early Christian Burial Chapel (14 Apáca Street)

During the excavations of 1968-1972 an apsidal burial building was unearthed in the yard of a dwelling-house in Apáca Street, in which three adults and a child had been buried under ground level. The last date of the multiple burials was defined by the coins found next to a bejewelled woman's remains: A.D. 385-390. The tomb was rebuilt in the 5th century. Above the tomb, a semi-circular bench and elevated base was built in the apse, and the floor of the burial chamber was also elevated. The later function of the building in the following centuries is unknown.

The uncovered graves can be seen under the modern protective building erected in the yard. The most spectacular finds of the rich material unearthed here are shown in photographs on the wall of the display building. The original ones are displayed at the exhibition of the Museum of Archaeology. Among those, a matching jug and drinking glass are of exceptional beauty, which are known to be early Christian symbols. Some of the many spindle-shaped, slim bottles used for storing scents or oils also can be seen here. The collection from the burial chapel also includes a large number of bronze, silver and gold jewellery and coins.

Turkish age

Gazi Kassim Pasha's mosque



The monumental building in the middle of Széchenyi square with its 23-metre dome and ogee windows dominates the square. Especially in the evening hours, lit by an inside glow, it attracts attention by its peculiar beauty.

The mosque is the biggest Turkish vestige in the country. There used to be an Early Christian tomb and perhaps a chapel in its place and a

Roman legionary's votive altar-stone was unearthed there as well. In the mid-13th century the St. Bartholomew parish-church was built here, which burned down in 1299. It was rebuilt in the 14th century, then during the invasion of the Turks, Pasha Gazi Kasim had it demolished in the late 1570s, and had a mosque and minaret raised partly of the old stones. After recapturing Pécs in 1686 the mosque was taken over by Jesuit monks. The minaret was dismantled in the beginning of the 18th century, and a bulky tower was built in its former place. The mosque was transformed into a baroque church, a new altar and oratories were built, and the dome was raised up. The exposition and reconstruction of the Turkish segments of the mosque began in 1938. An extension was added to the North-Western wall, so the interior space almost doubled. Between 1960-64, considering the requirements of monument preservation, the baroque dome was reconstructed in its original form. Since these last two modifications the exterior appearance of the mosque has not changed.

The interior of the church also offers a rich spectacle in the duality of Turkish vestiges and the disposition and ornaments of the Christian church. The niche of the mihrab belonged to the Turkish mosque, and the fragments of citations from the Koran still can be seen on the walls. The history of the church is recorded on the walls of the addition by Ernő Gebauer, a 20th-century artist of Pécs. The stained-glass windows of the vestry were created by Lili Sztéló, the excellent glass artist in 1938.

A contemporary eyemark of Széchenyi square is the campanile and St. Bartholomew's statue raised near the northern wall of the mosque in memory of the former St. Bartholomew's church and its martyr patron saint. The campanile is 13 metres high and it is made up of three gracile steel rods, with three different-sized bells. The martyrs' statue stands next to it with its symbols, the Rood and the snake. It was created by sculptor Sándor Rétfalvi of Pécs. The campanile is raised up only when bells are to ring, then it is drawn back down again so that it will not interfere with the spectacle of the mosque. The bells

chime meanwhile. The contemporary campanile music was composed by László Kircsi, Pécs. The design of the modern belfry is connected to Zoltán Bachmann, the architect-designer of Pécs.

The mosque of Jakovali Hassan Pasha

It is the most intact and conserved Hungarian mosque with minaret from the period of the 150-year Turkish invasion. It was built by the Yakova-born (today's Djakovo) Pasha of Pécs in the 16th century. The mosque has a square base, its dome is octagonal, and its minaret is 23 metres tall.



It was transformed into a Christian chapel in the early 1700s, and then it underwent several modifications in the following centuries. Its reconstruction as a monument began in 1955, and the Muslim place of worship furnished with the donations of the Turkish government was opened in 1975.

Entering the building, we are faced with the mihrab-chamber of the middle wall with its stalactite arches. Rich floral ornaments and quotations from the Koran can be seen on the walls and on the dome. The white and red stripes of the circular ornamentation of the dome is a reconstruction made after the remaining original fragments. It is worthwhile to observe the earthenware jugs placed in the walls and dome with their outward mouths, which were to provide excellent acoustics. These niches had been covered with a thin layer of plaster that was not replaced during the reconstruction for the sake of their spectacle. The flooring is covered with tiles from the Mecsek Hills, and it was made by the revealed fragments.

Idris Baba's turban-stone tomb



There used to be a Turkish cemetery on the southern slope of the Saint Roch (Rókus) Hill. The turbe is the tomb of Idris Baba and a Turkish pilgrimage destination. We know little about the person lying in the burial place. Turkish traveller Evlia Chelebi referred to him as a “faithful physician”, and according to Ibrahim Pechevi he was a miraculous seer. The octagonal, domed monument was

built in the 1500s. After the Turkish Invasion the building was taken over by the Loyolite order, and it was transformed into a plague hospital, then it was named after St. Roch, the patron saint of the plague-stricken (this memory is preserved

in the name of the hill). Later it was used as a powder-magazine by the army. It was partly uncovered and restored in 1912, but only got its present form in 1961 after its reconstruction. The burial space of Idris Baba cut into the rocks was also discovered, and his intact skeleton was found. The furniture, the sepulchral monument, the embroidered cover and the prayer rug was donated by the government of the Republic of Turkey. The tomb is a significant vestige of Turkish architecture in Hungary; Gül Baba's Mauseoleum in Buda is the other only known such monument. Both are Islamic destinations of pilgrimage.

Ruins of Memi Pasha's bath

Domed baths were essential parts of the Turkish townscape. They not only provided a place for people to bathe, but also a place for social meetings. The famous Turkish traveller Evlia Cselebi mentions three baths in Pécs in the second half of the 18th century: the baths of Pasha Memi, Pasha Ferhad and Pasha Quassim. The Bath of Pasha Ferhad was soon destroyed, only its foundation walls could be traced. The Bath of Pasha Memi was pulled down in the 1880s, but in 1963 it was restored.



Cathedral & Bishopric

St. Peter and Paul Cathedral

We have not much information concerning its first church, which might have been one of the Early Christian temples still standing at the time. The so called Illuminated Chronicle tells us that in 1064, when King Solomon was crowned in Pécs, the „bells fell down from the towers” owing to a fire that raged during the night following the coronation. This means that there was already a temple there which had to be reconstructed after the fire. The five-nave cross vaulted undercroft, built at the turn of the 11th and 12th centuries, still preserves its monumental embellished interior space. The church above it, built slightly later, is a three-nave basilica with no transept. Of its four towers two were constructed at the beginning and two other at the end of the 12th century. In the Middle Ages the interior of the church was richly decorated with stone carvings and frescos which were partly destroyed during the Turkish occupation then the repeated reconstructions of the following centuries covered them completely. The medieval ornaments were found as a result of the reconstruction carried out between 1883-1891. The stone carvings were then taken out from the wall and water colours were made about the remains of the frescos. The reconstruction kept the basilica architecture of the 12th century cathedral. The design was the

work of the Friedrich von Schmidt of Austrian, while the work was supervised by Ágoston Kirstein.



Similarly to the former Romanesque building, the cathedral, reconstructed in a Neo-Romanesque style, is a three-nave basilica with a flat ceiling, four towers and a ring of chapels. The rich paintings of its interior have their roots in the historicism of the 19th century. The walls and the ceiling are completely covered with paintings depicting various scenes

from the Bible and Hungarian saints. The paintings of the naves are the work of Karl Andreä and Moritz von Beckerath of Austria, while those in the chapels were made by Bertalan Székely and Károly Lotz. The figural carvings and the copies of the original ornaments of the undercroft descents were made by György Zala, while the relief above the southern gate and the apostle sculptures standing on the columns of the arcade are the work of György Kiss. These latter ones were replaced with the sculptures of Károly Antal in 1962-63. In the open space in front of the cathedral's gate the double bronze-gate composition of Sándor Rétfalvi was unveiled on December 30th in 2000. The outer bronze gate is decorated with leaves and clusters of grape on grapevine with birds and small lizards hiding among them. It also contains scenes recalling the foundation of the bishopric. The inner gate is embellished with 22 golden bronze high-reliefs depicting scenes from the Old Testament.

After its reconstruction the former basilica still reflects the magic of a medieval church. The cathedral with its four towers surrounded by the buildings of the Bishop's Palace, the Prebendal Cartulary and Presbytery and the Mediterranean square in front of it is the best sight of the town and an everlasting memory that visitors may take home.

The remains of Janus Pannonius (1434-1472), the Renaissance poet and former bishop of Pécs were discovered when restoring the cathedral in 1991. The leaders of the bishopric assumed that the remains belonged to the late bishop and the results of an anthropological research received in the spring of 2008 confirmed that their suspicion had been correct. In the autumn of 2008 the former bishop was laid to rest in the undercroft of the cathedral in the form of a solemn ceremony. The remains of the great poet are deposited beside those of bishop Nándor Dulánszky.

Cathedral Museum



During the rebuilding of the Cathedral between 1883-1891, the figural, coloured stone carvings were found that had adorned the original walls of the church built in the 12th century. The former church had suffered serious damage during the Turkish invasion (16th century). In spite of that, the troves possess a remarkable artistic value. During the 19th-century

restoration the damaged carved stones were not wished in their original place, therefore they were deposited in the granary of the Cathedral. Later they were stored in the corridors and some rooms of the bishop's library, then in a basement room of the Cathedral, so they could not be seen by the public. A foundation was established for the construction of the Cathedral Museum and the restoration of the stonework in 1990. As a result of the work beginning in 1994, the most beautiful ornaments of the Romanesque cathedral can now be seen in the stone repository opened in 2005.

In the grand space six hundred pieces out of the nearly thousand-piece collection can be seen at the exhibition. In their arrangement and prospect those ornaments have a central role that were brought to the surface in bigger and more coherent units, such as the popular altar chapel and the relief ornaments of the undercroft descents. Their arrangement reconstructs their original, medieval place and role. Beside the Romanesque stonework, the exhibition displays stone artefacts from later eras of the cathedral as well, such as fragments from 14th-century carvings. These include the key-stone with the heads of the Apostles, the figure of St. George with the dragon, the Holy Spirit with the dove, and the plaited, palmette and grapelike ornaments, column-fragments and headstones can also be admired by visitors.

The Cathedral stone repository can evoke the former entirety of our cultural heritage that has left us with these fragments of the European art of medieval church-architecture after thousand years of hardships.

The upstairs gallery provides a place for periodic historical, art and crafts exhibitions.

Bishop's Wine Cellar

In the cellar built by Bishop Ferenc Nesselrode in the 1700s the wines of 4 wine regions (Pécs, Tolna, Szekszárd, Villány) located in the area of the Pécs diocese are treated and bottled. The tasting room above the cellar, having a seating

capacity of 100 offers 15-20 different wines. Part of the cellar is an exhibition space featuring the traditional grape processing and wine making equipments.

Zsolnay heritage

ZSOLNAY PÉCS – these were the two words that Vilmos Zsolnay would write and stamp on the products of his factory from the beginning. He kept the name of the city in his logo even when he changed the shape of his stamp. His successors followed this tradition. The Zsolnay family and the subsequent directors of the factory indicated their affection towards the city in several ways, while the citizens of Pécs have always respected the “Zsolnay” and are still proud of it.

Zsolnay and Pécs, it is not only the name but also the image and the activities of the factory and the city that have always been closely related. Five successive generations of the Zsolnay family have enriched the culture of the city and added to its wealth. Wherever we walk in the city we can encounter the heritage of the Zsolnay family everywhere: on the facade of old and new houses, on roofs, on sculptures and reliefs, in shop-windows, on commemorative plaques and in the exhibition of the 55-year-old Zsolnay Museum introducing the complete history of the factory. Thanks to the “2010 European Capital of Culture“ programme we can also get a taste of this great heritage in the historic buildings of the Zsolnay Cultural Quarter established on the site of the former manufactory where we can also visit the Gyugyi Collection introducing the works of the factory from the periods when they produced historicist and Art Nouveau ceramics.

The Zsolnay Cultural Quarter



The Zsolnay Cultural Quarter is the gem of Pécs. The heritage of the former world renowned ceramics factory of the Zsolnay family lives on under worthy circumstances as the new cultural centre of the city.

During the course of the past few years an outstanding and unique investment project was realized that resulted in creating a new cultural “city” within the city. The still active parts of the porcelain factory were all moved into the eastern part of its premises so the emptied buildings provide space for such cultural and artistic venues that are not only new patches of colour on the touristic palette of Pécs but they also enrich both locals and visitors with a set of institutions that offer a large variety of activities to spend their free time. These outstanding cultural venues and spectacles of Pécs make up an area of 50,000 square metres of the former manufactory that was fully rebuilt and renovated.

Visiting the exhibitions or just simply walking around the area and taking it all in is a full day's programme that grabs and carries the attention of all the members of the family.

Exhibitions, cafés, restaurants, shops, a university quarter, concert and conference halls, the Visitor Centre, the Live Manufacture and the Interactive House of Playful Sciences, a planetarium, a Zsolnay gift shop, several open-air playgrounds and a basketball court – this is the Zsolnay Cultural Quarter today; the legend of Pécs reborn awaiting all age groups seeking creative experience and an exciting cultural adventure, just a 15-minute-walk away from the city centre.

The Zsolnay family and factory history exhibition



The figure of Vilmos Zsolnay is not emblematic only in Pécs. The influential figure of the Hungarian ceramics industry made the Zsolnay brand and the achievements of the high quality national industry well-known over the borders of Hungary too. The Zsolnay family and factory history exhibition gives an insight to the visitor of the most precious moments of the

life of the industrial dynasty starting with the simplest industrial ceramic items to the most decorated ornamental pieces and the life-changing family events.

Golden Age of Zsolnay Exhibition

Thanks to the sacrifices of the city the collection of László Gyugyi, the Hungarian collector living in the United States, has found its place in the Zsolnay Cultural Quarter. The collection contains the best historicist and Art Nouveau ceramics that were on display at various world's fairs.



According to the wish of the collector this 600-piece exhibition, called “The Golden Age of Zsolnay”, can be seen in the former dwelling-house of the Sikorski family located inside the Zsolnay Cultural Quarter. This was the place from where these products departed to conquer the world.

Live Manufacture

The Zsolnay Live Manufacture – porcelain in the making is the special venue of the Zsolnay Cultural Quarter where the visitors can see the more than 150-year-old production processes, popular motifs and products of the famous porcelain manufacture.

Pink Zsolnay Exhibition

The exhibition entitled „In the beginning was the pink...” aims to introduce the bests of the Zsolnay objects to the visitors.

Zsolnay Mausoleum

After Vilmos Zsolnay, founder of the Zsolnay factory passed away in 1900 his son had the mausoleum erected right next to the factory on



top of a little hill that had been the scaffold of the city before. The venue was not important for the family because of its shady past.

The small hill used to be a dear place of the founder of the factory where he had spent a lot of time just glazing down at the factory lying underneath. According to the plans of the son-in-law of Vilmos Zsolnay; Tádé Sikorski the construction

works of the factory and the landscaping of the surrounding area had began exactly 100 years ago, in 1901. All the workers of the factory have taken part in building the Pécs Pantheon; they have worked out each and every little detail together. „... the family had all the bricklayer, carpenter, blacksmith ...etc works carried out by the colleagues using the raw materials of the factory and the people working on the chapel are still mainly those who had served the old man with faith and love.” - reports the Pécsi Napló about the event in 1901.

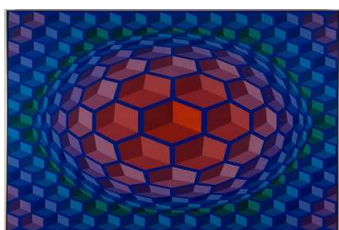
The ore coffin of Vilmos Zsolnay was put to its eternal rest in the crypt of the family in 1913, and he was followed by his wife Terézia Bell in 1919. The only other person lying in the crypt today is their son Miklós because the mortal remains of the other family members have fallen victim to the vandal destructions after which they were reburied in the Pécs Cemetery of Honour in damaged state in 1986.

The neo-roman building includes a burial chapel and a burial chamber underneath with a decorated eosin sarcophagus and 32 coffin vaults. The facade of the mausoleum had been covered by unenameled pyrogranite tiles while the hemispheric dome had been covered by dark green majolica-glazed shaped tiles. An altar and an eternal light were placed inside the chapel the walls of which are decorated by colourful tiles. The glasses of the round windows were



originally produced in the Roth workshop. On the inside surface of the mausoleum the blue sky, cherubs and golden stars watch the sleep of the deceased while secessionist decorations and flower strings overwhelm the space by an inimitable serenity. The full inside decoration was the work of the leading sculptor of the factory; Sándor Apáti Abt. In the middle of the chapel is the bluish glazed opeion hole with a Roman column parapet through which one can look down into the sepulchral vault. On a podium in the middle of the vault lies the eosin sarcophagus of Vilmos Zsolnay decorated on all sides by figural scenes. This architectural division is characteristic to the Paris burial site of Napoleon where people looking down from above bow their heads for the deceased while in the crypt they look up to the sarcophagus that is placed on a podium. Whoever spends some time here unconsciously gives respect to those of its resting inhabitants. They say that during the time of the winter solstice when the sun is at its zenith the light coming in unravels the secret of the eosin. By paying a little attention we might become the knowers of the secret...

During the storms of history the building and its surroundings have fallen victim of constant destruction and the ceramic building elements were scattered. The full renovation of the mausoleum - except for the roofing - has been done in the framework of the Pécs2010 European Capital of Culture Programme. It included not only the renovation of the building but the promenade leading up to it with the lions and the fence that needed to be rebuilt fully from scratch based on some early photos.



Museums

Vasarely Museum

Vasarely gave 42 serigraphs (screen-prints) to the museum in 1968. This series was displayed at the first Vasarely exhibition in Hungary. Further donations - paintings, tapestries, plastic and graphic pieces - arrived here the following year, with the purpose of establishing the Vasarely Museum. The artist gave the city of Pécs not only his own works, but some valuable pieces by his wife Claire and his son Yvaral and other contemporary European artists. The exhibition of Vasarely Museum opened in the restored and transformed birth-place of the artist under 3 Káptalan Street in 1976. Thus, Western European ideological streams were officially accepted by Hungarian cultural politics. The exhibition - one of the most popular and visited ones in Pécs - was shown in several neighbouring countries during the last decade, therefore the region could get acquainted with Vasarely's work.

The collection of the Museum reflects on defined, significant stages of the artist's life-work from the 1940s. The exhibits show the different periods of Vasarely's versatile genres and techniques which are connected to personal experience or environmental surroundings. Visitors are surprised to see the anaglyphic,

pulsating compositions of the “Vega” group. The waving line-pattern of the tapestry “Zebras” (1960) appeared as early as in the 1930’s in his early experiments.

Besides Vasarely’s life-work, the Museum also exhibits his wife Claire’s and his son Yvaral’s works.

Csontváry Museum

The paintings by Tivadar Csontváry Kosztka, deceased at 66, were left behind his studio in Budapest. His heirs offered large-sized paintings on sale for nearby carriers, thinking the excellent quality canvasses could be used as car covers.



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the

Gedeon Gerlóczy, a young architect just finishing his studies, was looking for a studio, and catching sight of the advertisement on the door, took a look at Csontváry’s deserted atelier. One of the rolled-up paintings uncurled by accident, and Gerlóczy was faced by the “Lonely Cedar” that - as he told later - had an incredible impact on him. During the auction sale held the next day, he managed to buy up the bequest in advance of the bidding carriers. The paintings were waiting for their chance packed in crates for a while then. Gerlóczy, who was teaching at the Arts college, managed to place some large-sized pieces in the rooms of the College. After the exhibitions in Paris and Brussels in 1949 the paintings were moved to the basement of the National Museum of Arts, and some of them were given back to the owner only six years later. Later on the masterpieces were kept in the research rooms of the National Gallery; one of the large paintings was leaned to the wall in the corridor - facing the wall. When Pécs asked the ageing Gerlóczy’s permission to show the paintings at a permanent exhibition in the early 1970s, he agreed. The Csontváry Museum was established by a deposit contract of ten years.

The museum was opened in 1973, on the 120th anniversary of the artist’s birth - first with eight paintings exhibited in a single room and with a scarce selection of early sketches. The exhibition expanded significantly ten years later, when the state of Hungary bought Gedeon Gerlóczy’s collection that was moved to The Csontváry Museum with the exception of four paintings. The exhibition was enriched with paintings made in Dalmatia, Southern Italy and at home, in Hortobágy and Selmecebánya (today’s Banská Štiavnica). One of the most significant masterpieces, the beautiful “Lonely Cedar” can also be found here, which was painted as a symbolic portrayal of the artist himself.

Zsolnay Museum

The exhibition introduces the best products of the factory from its first great success at the World's Fair in Vienna (1873) to the latest vases and ornamental pots. The personal belongings on display in the Zsolnay memorial room recall the everyday life of this respected family. Miklós Zsolnay, a merchant, founded a stoneware factory in Pécs in 1853. It was his son, Vilmos Zsolnay who developed this small manufactory into a world famous factory. Beginning from the 1870s till the end of the century, Teréz and Júlia, the two daughters of Vilmos Zsolnay, also took part in the art and design activities. In 1898 young artists established an Art Nouveau workshop within the factory, which played an important part in the art life of the city, too. After the extended experiments of Vilmos Zsolnay, in 1893, the factory began to produce its ornamental pots having a polychromatic and metallic luster glaze that is called „eosin”. After the death Vilmos Zsolnay in 1900, his son Miklós began to manage the already renowned factory, which gained high reputation overseas, too. This was the time when architectural ceramics, whose several excellent examples can be seen in the centre of Pécs, became popular and highly marketable.

More information: www.visitpecs.com

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