

14th International Symposium “Spectroscopy in theory and practice”

Final Program:

Sunday, April 10, 2005

12:00 – 16:00 Registration (Hotel Perla, 14 ISSTP registration desk)
16:00 Opening of the 14 ISSTP (Pinta conference hall)

Spectroscopy of biological membranes (Pinta conference hall)

Chairpersons: M. Schara, S. Passamonti

Plenary lecture:

16:30 - 17:15 (PL1) **P. Laggner**: Bridging the Nano-gap: Simultaneous small angle scattering and powder diffraction

Oral communications:

17:15 – 17:45 (KN1) **I. Serša**: Spatially selective NMR spectroscopy
17:45 – 18:00 (O1) **I. Dogša, P. Laggner, J. Štrancar, D. Stopar**: Small-angle X-ray scattering (SAXS) investigation and structural modelling of bacterial extracellular polysaccharides (EPS)
18:00 – 18:15 (O2) **M. Prezelj, J. Osredkar, M. Krsnik, M. Schara, A. B. Kobal**: Reduced and oxidized glutathione in blood samples of miners
18:15 – 18:30 (O3) **M. Milatovič, S. Pečar, M. Nemec, M. Hren, B. Žegura, M. Filipič, J. Žel, M. Schara**: The effect of paclitaxel on plasmalemma of human breast cancer cells
18:30 – 18:45 (O4) **K. Šturm, A. Kristl, M. Schara**: The mathematical model for drug diffusion across rat jejunum in vitro
19:00 Get together (Hotel Perla, Conference centre)

Monday, April 11, 2005

Molecular spectroscopy (Pinta conference hall)

Plenary session

Chairpersons: J. Kidrič, P. Laggner

8:30 - 9:15 (PL2) **C. Luecke**: Intracellular lipid binding proteins: evolutionary development of structure and function
9:15 - 10:00 (PL3) **J. Eckert**: Applications of inelastic neutron scattering vibrational spectroscopy to problems in heterogeneous catalysis

10:00 - 10:30 Coffee Break

Molecular spectroscopy (Pinta conference hall)

Oral communications:

Chairpersons: C. Luecke, U. Lavrenčič-Štangar

- 10:30 - 11:00 (KN2) **V. Smrečki, N. Müller:** Theoretical simulation of conformational influence on NMR chemical shielding anisotropy
- 11:00 - 11:30 (KN3) **P. Pristovšek:** Structural approach towards endotoxin inhibition by peptides
- 11:30 - 12:00 (KN4) **C. Thibaudeau:** NMR and DFT studies of O-glycoside and hydroxymethyl group conformation in mono- and disaccharides
- 12:00 - 12:30 (KN5) **P. Judeinstein:** Multi-scale description of ionic conductivity mechanisms in polymer electrolytes

12:30 - 14:30 Lunch Break

Atomic spectroscopy (Pinta conference hall)

Plenary session:

Chairpersons: T. Kantor, R. Milačič

- 14:30 - 15:15 (PL4) **J. I. Garcia-Alonso:** Determination of butyltin compounds in environmental samples by isotope dilution mass spectrometry
- 15:15 – 16:00 (PL5) **H. Becker- Ross, S. Florek, U. Heitmann, H. D. Mao, M. Okruss:** High-Resolution CS-AAS – a new powerful tool for element analytics

16:00 - 16:30 Coffee Break

Oral communications:

Chairpersons: C. Sarzanini, J. Štupar

- 16:30 - 17:00 (KN6) **T. Kantor, G. de Loos-Vollebregt:** Sample introduction with electrothermal vaporization for ICP-OES/MS
- 17:00 - 17:20 (O5) **B. Kralj, R. Milačič, I. Križaj, P. Bukovec:** Speciation of aluminium in tea infusions
- 17:20 - 17:40 (O6) **T. Zuliani, G. Lespes, M. Potin-Gautier, P. Bukovec, R. Milačič, J. Ščančar:** Contamination of sewage sludge with organotin compounds
- 17:40 - 18:00 (O7) **B. Koklič, M. Veber:** Influence of shape of sampling mould to the homogeneity for analysis of Cu-Ti-Zn alloy

Poster session:

18:00 - 19:00

All posters are displayed throughout the symposium. Authors of posters **P1 – P35** must be present at their poster during this session.

Tuesday, April 12, 2005

Gamma spectroscopy and nuclear related methods

Chairperson: A. R. Byrne

Plenary lecture:

8:30 - 9:15 (PL6) **M. Hult**: Underground gamma-ray spectrometry

Oral communications:

9:15 – 9:30 (O8) **T. Vidmar, M. Korun, A. Likar**: Close-geometry detector efficiency calibration with a Co-60 point source

9:30 – 9:45 (O9) **R. Jaćimović, A. Trkov**: A new k0_IAEA software for neutron activation analysis: advantages and disadvantages compared to the kayzero/solcoi program

9:45 – 10:00 (O10) **Z. Jeran**: The use of nuclear methods to monitor air pollution

10:00 – 10:15 (O11) **U. Repinc, L. Benedik, R. Jaćimović**: Comparison of RNAA and INAA for determination of short-lived radionuclides in biological materials

10:15 – 10:30 (O12) **L. Benedik, A. Alonso, A. Timotheos, H. Kühn, A. Moens, A. Stolarz, A. Verbruggen, R. Wellum**: Nusimep-5: Uranium and plutonium isotopic mixtures in saline samples

10:30 - 11:00 Coffee Break

Chemometrics

Chairperson: M. Novič,

Plenary lecture:

11:00 – 11:45 (PL7) **S. C. Basak**: Applications of chemodescriptors and biodescriptors in biological structure – activity relationships

Oral communications:

11:45 – 12:10 (KN7) **I. Kuzmanovski, A. Madevska-Bogdanova, M. Trpkovska**: Multicategory support vector machines for classification of human urinary calculi

12:10 – 12:35 (KN8) **S. Erić, T. Šolmajer, J. Zupan, M. Novič, M. Oblak, D. Agbaba**: The application of chemometric tools in quantitative structure-activity relationships studies of alpha₁ adrenergic antagonists

12:35 – 13:00 (KN9) **N. Ogrinc, I. J. Košir, M. Kocjančič, J. Kidrič**: Determination of the geographical origin and authenticity of wine by chemometric methods based on multi-site isotopic variables

13:00 - 14:30 Lunch Break

Mass spectrometry

Chairpersons: D. Žigon, M. Rožman

Plenary lecture:

14:30 – 15:15 (PL8) **D. Barcelo, M. Petrović, M. J. Lopez de Alda, M.D. Hernando:** LC-MS-MS of selected organic pollutants in the aquatic environment

Oral communications:

15:15 – 15:45 (KN10) **L. Klasinc, S. Kazazić, D. Srzić:** Gas phase ligation of metal monocations with PAH and heteroanalogs
15:45 – 16:05 (O13) **A. Wallace, M. Kennedy, S. Pringle, I. Campuzano, T. McKenna, J. Castro-Perez, S. Preece, J. Langridge:** Novel approaches for the enhancement of sensitivity and dynamic range on a hybrid quadrupole orthogonal acceleration time-of-flight mass spectrometer

16:05 - 16:30 Coffee Break

Oral communications:

Chairpersons: L. Klasinc, D. Barcelo

16:30 – 16:50 (O14) **M. Kovačević, S. Andrenšek:** Fragments of organic molecules in ICP-MS
16:50 – 17:10 (O15) **M. Rožman:** Gas phase H/D exchange of sodiated amino acids: why do we see zwitterions?
17:10 – 17:30 (O16) **T. Kosjek, E. Heath, B. Kompare:** Degradation of pharmaceuticals in a pilot sewage treatment plant by GC-MS
17:30 – 17:50 (O17) **C. Somerton, O. Wilkin, T. Brockwell, J. Morrison, A. Phillips:** New methodology in continuous flow IRMS

Poster session:

18:00 - 19:00 All posters are displayed throughout the symposium. Authors of posters **P36 – P67** must be present at their poster during this session.

20:00 Symposium dinner

Wednesday, April 13, 2005

Plenary session:

Chairpersons: P. Trebše, I. Arčon

- 9:00 – 9:45 (PL9) **M. Sarakha:** Degradation of aromatic pesticides by homogeneous and heterogeneous photocatalysis: from the primary processes to mineralisation
- 9:45 – 10:30 (PL10) **R. Frahm:** QEXAFS: Time dependent in situ studies of atomic structure and chemical state

Laser spectroscopy

Chairpersons: M. Terzić, M. Franko

Oral communications:

- 10:30 – 10:45 (O18) **D. D. Markushev, M. V. Rabasović:** Calibration of pulsed photoacoustic systems for highly excited polyatomic molecules
- 10:45 – 11:00 (O19) **D. M. Todorović, V. Jović, M. Smiljanić, T. Grozdić:** Photoacoustic spectroscopy: Investigation of the Na-ion defect states in SiO₂-Si system
- 11:00 – 11:15 (O20) **J. Kožar-Logar, A. Malej, M. Franko:** Thermal lens spectrometry in studies of phytoplankton pigments

11:15 - 11:45 Coffee Break

X-ray spectroscopy and related techniques

Chairperson: P. Barbieri, J. Padežnik Gomilšek

Oral communications:

- 11:45 – 12:15 (KN11) **P. D' Angelo:** New developments in the quantitative structural analysis of XAS spectra
- 12:15 – 12:30 (O21) **A. Kodre, J. Padežnik Gomilšek, I. Arčon, A. Meden, D. Mihailović:** Specific EXAFS tools in analysis of MOSI nanowires
- 12:30 – 12:45 (O22) **L. Armelao, H. Bertagnolli, S. Gross, V. Krishnan, U. Lavrenčič Štangar, K. Müller, B. Orel, G. Srinivasan, E. Tondello, A. Zattin:** Spectroscopic methods for the investigation of mixed oxide materials: a multitechnique approach
- 12:45 – 13:00 (O23) **A. Ristić, I. Arčon, N. Novak Tušar, V. Kaučič:** Spectroscopic investigation of redox activity of microporous iron aluminophosphate
- 13:00 – 13:15 (O24) **N. Novak Tušar, N. Zabukovec Logar, M. Mrak, G. Vlačić, I. Arčon, V. Kaučič:** Local environment of titanium in microporous/mesoporous composite
- 13:15 – 13:30 (O25) **I. Arčon, J. T. van Elteren, H. J. Glass, A. Kodre, Z. Šlejkovec:** Analysis of As-contaminated soil by XAS spectroscopy
- 13:30 Closing
- 15:00 Excursion

List of posters:

- P1 **Z. Rimpapa, E. Sofić, A. Šapčanin, J. Toromanović, I. Tahirović:** Inhibition of neutral red photolysis with different antioxidants
- P2 **K. BenTayeb, A. H. Al-Taiar, H. Ilikti:** Spectrophotometric studies of amines complexes with metal ions
- P3 **T. Dramićanin, M. Dramićanin, B. Dimitrijević, V. Jokanović:** Discrimination between normal and malignant breast tissues by synchronous luminescence spectroscopy
- P4 **J. Savić, V. Vasić:** Complex formation between Pd(II) and immobilized imidazol-azo-chromotropic acid
- P5 **V. Vasić, M. Čakar, G. Popović, T. Momić:** Spectrophotometric study of quercetin stability in various media
- P6 **M. Kračun, S. Borišek, D. Kocjan:** ^1H and ^{13}C NMR study of atorvastatin and some analogues
- P7 **V. Guzsány, J. Csanádi, F. Gaál:** NMR study of the influence of pH on the persistence of some neonicotinoides in water
- P8 **S.C. Basak, R. Natarajan:** NMR spectral invariants as numerical descriptors for diastereomers and enantiomers
- P9 **U. Černigoj, U. Lavrenčič Štangar, P. Trebše, B. Orel:** Comparison of UVA absorption of different TiO_2 films and their photocatalytic properties
- P10 **S. Vajnhandl, A. Majcen Le Marechal:** Sonochemical decolouration of reactive azo dye Reactive black 5
- P11 **U. Lavrenčič-Štangar, J. Eckert, J. Vince, J. M. Zanotti, B. Orel, S. Hočevar:** Quasielastic neutron scattering studies on proton conducting ormosil membranes
- P12 **S. Dobrinas, S. Birghila, V. Coatu:** Determination of some organochlorine pesticides and Cu, Cd, Pb in honey
- P13 **Ž. Nikitović, A. Strinić, V. Šamara, G. Malović, Z. Petrović:** Emission coefficients in helium
- P14 **S. Batovac, K. Hafner, E. Rudžia, J. Pašalija:** Determination of ambient mercury using atomic absorption spectrometry-cold vapours technique
- P15 **S. Bukvić, V. Žigman, A. Srecković, S. Djeniže:** Measured Stark widths and shifts of the 251.328 nm and 252.569 nm Ar IV spectral lines
- P16 **V. Popescu, S. Birghila, S. Dobrinas:** Determination of Fe, Mn, Zn, Pb in garden flowers (blue hyacinth and chrysanthemum)
- P17 **E. Chirila, I. Carazeanu, D. Sava, N. Lupascu:** Determination of trace metal concentrations in algae from different biotopes in the Romanian Black seacoast by the use of FAAS
- P18 **R. Bregar:** Boron in underground water on the area of the city of Ljubljana
- P19 **A.R. Tančić, M. R. Nikolić:** Post collision interaction and the line form in the Auger electron spectra
- P20 **V. Jokanović, M. Dramićanin, Ž. Andrić:** Nanodesigning of SiO_2 : Eu^{3+} particles obtained by spray pyrolysis method and their luminescence properties
- P21 **L. Husáková, J. Šrámková, M. Barinová:** The use of chemical modifiers for direct determination of cadmium and lead in human urine by ETAAS with deuterium background correction
- P22 **B. Podkrajšek, J. Turšič, P. Kralj, I. Grgić:** Particle size distribution of some metals in aerosols collected at two different urban locations
- P23 **I. Božič Carli, I. Grabec Švegl:** Metrological study of the mass fraction measurements of gold and platinum in precious metal alloys by ICP-AES: traceability schemes
- P24 **B. Križanec, E. Vončina, A. M. Le Marechal, D. B.-Vončina:** Optimization of a GC-MS/MS (ion trap) method for the analysis of organotin compounds in water samples
- P25 **M. Islamčević-Razboršek, V. Doleček, D. B. Vončina, E. Vončina:** Determination of some derivatised terpene acids in rosemary (*rosmarinus officinalis L.*) by GC-MS
- P26 **I. Kralj Cigić, H. Prosen:** Assessing the authenticity of black tea aroma by GC-MS
- P27 **D. Vidic, M. Maksimović, S. Čavar, M. Miloš:** Determination of chemical constituents of the essential oil from two micromeria species
- P28 **P. Cuderman, E. Heath, L. Zupančič-Kralj:** Determination of personal care product residues in aqueous samples
- P29 **T. Gostič:** Investigation of samples from clandestine laboratory - cocaine in polymethyl methacrylate (PMMA) resin

- P30 **R. Grahek, A. Kocijan:** Structure determination of tamsulosin impurities by tandem mass spectrometry
- P31 **B. Mozetič I. Tomažič, A. Škvarč, P. Trebše:** Determination of white grape cv. rebula polyphenols
- P32 **A. Jemec, B. Mozetič, T. Tišler, P. Trebše:** HPLC-DAD determination of imidacloprid stability for application in toxicity tests
- P33 **S. Geromanos, K. Richardson, P. Young, R. Denny, K. Neeson, T. McKenna, C. Doreschel, M. Gorenstein, G. Z. Li, T. Riley, J. C. Silva, J. Langridge:** A novel qualitative and quantitative LC/MS based approach to protein profiling and biomarker discovery
- P34 **J. Brown, D. Kenny, E. Claude, R. Bateman:** A parallel approach to post source decay MALDI-TOF analysis
- P35 **M. Snel, E. Claude, D. Kenny, T. McKenna, J. Langridge:** Parallel PSD analysis of 2D-gel spots from *e.coli*
- P36 **A. Vidic, Z. Ilić, D. Deljković, U. Repinc, R. Jakopič, L. Benedik, S. Marić:** The activities of Uranium radioisotopes in water samples from Bosnia and Herzegovina
- P37 **S. Petrović, A. Leskovac, G. Joksić:** Cytotoxicity of low doses of ionizing radiation measured by flow cytometry
- P38 **R. Jakopič, L. Benedik:** Comparison of various dissolution methods for determination of uranium isotopes in contaminated samples
- P39 **P. Tavčar, L. Benedik:** Radioanalytical procedure for characterisation of radioactive wastes
- P40 **O. Čuknić, A. Kandić:** The whole body counter at Vinča institute
- P41 **A.B. Kandić, I.S. Vukanac and D.J. Todorović:** Determination of the linear attenuation coefficients in the different matrices
- P42 **D. Novković, L. Nađđerđ, A. Kandić and I. Vukanac:** The experimental testing of the digital multichannel analyzer
- P43 **M. Gajić-Kvaščev, M. Eremić-Savković, V. Andrić:** Comparison of measured and simulated gamma spectra from environmental samples
- P44 **A. Osterc, V. Stibilj:** Development of a method ¹²⁹I determination
- P45 **D. Popović, D. Todorović, M. Radenković:** Ground level air radioactivity monitoring by gamma spectroscopy
- P46 **J. Vaupotič, I. Kobal:** Radon doses in Slovenian schools based on alpha spectrometry
- P47 **S. Klemenc:** Selection of metric for the comparison of heroin samples by FTIR spectroscopy
- P48 **N. Grošelj:** Optimization of neural networks by simplex method
- P49 **D. Brodnjak Vončina, M. Novič, N. Mirkovič, E. Vončina:** Monitoring of underground waters and chemometrics characterization of samples from different wells
- P50 **S. Dragović, A. Onjia, G. Bačić:** Implementation of neural networks for classification of moss and lichen samples on the basis of gamma spectrometric analysis
- P51 **Š. Župerl, G. Mlinšek, M. Novič, T. Šolmajer, J. Zupan:** Prediction of thrombin and trypsin inhibition constants based on neural networks and genetic algorithm
- P52 **E. Boriani, M. Spreafico, E. Benfenati, M. Novič:** Modeling of binding affinities of ligands to estrogen alpha and estrogen beta receptors
- P53 **A. Karawajczyk, S. Passamonti, N. Medič, O. Ganyiu, V. Drgan, M. Novič:** The interaction of poliphenolic compounds with bilitranslocase described by counterpropagation neural network
- P54 **S. Passamonti, M. Terdoslavich, A. Margon, A. Cocolo, N. Medic, G. Decorti, M. Franko:** Bilirubin analysis by thermal lens spectrometry: A tool to investigate the molecular mechanism of its membrane transport
- P55 **M. Terzić, D. D. Markushev, M. Rabasović:** Multiphoton processes in gas mixture: relaxation mechanisms
- P56 **M. Stanković, G. Joksić, M. S. Trtica:** IR laser-induced changes to plant tissue: Onion epidermis (*Allium cepa*)
- P57 **M. Bavcon Kralj, M. Franko, P. Trebše:** Determination of oxidation efficiency of OPS using AChE biosensors and GC-MS technique
- P58 **D. A. Nedosekin, M. Y. Kononets, M. A. Proskurnin:** Thermal-lens study of surface-absorbing glasses and polymers
- P59 **D. A. Nedosekin, S. N. Bendrysheva, M. A. Proskurnin, W. Faubel, U. Pyell:** Indirect thermo-optical detection in capillary electrophoresis

- P60 **M. Novič, B. Križ, D. Günther:** Laser ablation-ICP-MS-based analysis of selected archaeological objects
- P61 **D. Horvat, M. Terzić, J. Možina:** Determination of optodynamic excitation mechanisms following laser pulse absorption in CuSO₄ solution
- P62 **A. Ahmedova, V. Rusanov, A. Hazell, J. Wolny, M. Mitewa:** ⁵⁷Fe Mössbauer study on a Fe(III) complex of 2-acetyl-1,3-indandione
- P63 **M. Tasić, B. Đurić-Stanojević, S. Rajšić, Z. Mijić, V. Novaković:** Physico-chemical characterization of PM₁₀ and PM_{2.5} particles in the Belgrade urban area
- P64 **P. Barbieri, F. Cozzi, L. Capriglia, I. Pellegrini, B. Kaulich, M. Salome, E. Reisenhofer:** Further steps in X-ray microscopy studies on air particulate
- P65 **J. Padežnik Gomilšek, I. Arčon, A. Kodre:** Atomic effects in Iodine K-edge EXAFS analysis of redox I⁻/I₃⁻ solid-state electrolytes
- P66 **A. Müllner, I. Arčon:** Xanes determination of Fe valence state with a laboratory X-ray source
- P67 **K. Maver, I. Arčon:** Systematic errors in EXAFS analysis