15th
Informal Meeting on Mass Spectrometry
Smolenice 12-16 May 1997

organized by:

CHEMICKÝ ÚSTAV, SLOVENSKÁ AKADÉMIA VIED,
BRATISLAVA, SLOVAK REPUBLIC

MAGYAR TUDOMÁNYOS AKADÉMIA,
KÖZPONTI KÉMIAI KUTATÓ INTÉZETE,
BUDAPEST, HUNGARY

CONSIGLIO NAZIONALE DELLE RICERCHE,
AREA DI RICERCA DI PADOVA, ITALY

Organizing Committee

Chairman: V. Kováčik
Vice-Chairman: P. Traldi, K. Vékey
Secretary: G. Kogan
Members: M. Kačuráková, J. Königstein, V. Pátoprstý
Technical Assistance: E. Kanský
Monday, May 12, 1997

10:00 - 14:00 Registration

12:30 Lunch

13:50 - 14:00 Opening

Chairman: J. Beynon

L1 14:00 - 14:45 E. R. Schmid
Recent Developments in Mass Spectrometry

L2 14:45 - 15:30 R. J. Cotter
Time-of-Flight Mass Spectrometry: Developing an Important New Technology for Chemical/Biological Research

L3 15:50 - 16:35 P. J. Derrick
Fourier-Transform Ion Cyclotron Resonance and Electrospray Ionisation

L4 16:35 - 17:20 D. Favretto

L5 17:20 - 17:40 A. M. Gioacchini
A Comparison of Analytical Performance of SDS-page, ESI-MS and Maldi-TOF-MS in the Study of the Protein Extract from Jararaka Snake Venom

L5B 17:40 - 18:00 V. Raverdino
Advantages of the Orthogonal Spray Geometry for an API-Electrospray Ion Source for LC-MS and LC-MSn

19:30 Dinner

20:00 - 21:30 Informal get-together party
Tuesday, May 13, 1997

8:00  Breakfast

Chairman: R.J. Cotter

L6  9:00 - 9:45  C. Fenselau
    Metal Ion Flux in Metalloprotein Chemistry

L7  9:45 - 10:30  E. Gelpí
    Determination of Pesticide Epitopic Density in Protein Immun conjugates by Electrospray Mass Spectrometry

L8  10:50 - 11:35  V. Reinhold
    Carbohydrates and Microbial Surfaces: Studies by ESI-MS and CID

L9  11:35 - 12:20  J. Thomas-Oats
    Structure-Function Studies of Biological Signal Molecules: A Mass Spectrometric Approach

L10 12:20 - 12:40  L. Brüll
    Loss of Internal Monosaccharide Residues from Underivatised and Per-O-methylated Trisaccharides

12:30  Lunch

Chairman: M. Claeys

L11  14:00 - 14:45  F. De Angelis
    Lignins: A World of Problems and the Contribution of Mass Spectrometry to Solve Them

L12  14:45 - 15:30  D. Kuck
    Recent Results on the Gas-phase Chemistry of Protonated Alkylbenzenes

L13  15:50 - 16:10  K. Pihlaja
    Electron Ionization Mass Spectra and Exo-Endo Isomerization of a Double Bond in the Addition Products of Cycloalkylidene Malonic Acid Derivatives and Push-Pull Alkenes
L14 16:10 - 16:30  F.J. Winkler  
Detection of Chiral Supramolecular Propellers of Dialkyltartrate Trimers with Alkali Ions by ESI MS

16:30 - 17:15  Poster Session I - Oral presentation

17:15 - 19:00  Poster Session I

IP1  L. Rovatti  Liquid Chromatography/Electrospray Tandem Mass Spectrometry of Methylated Purine Bases

IP2  Y.L. Ma  Characterization of Flavone and Flavanol Aglycones by Collision-Induced Tandem Mass Spectrometry

IP3  P. Traldi  Fast Atom Bombardment in the Characterization and Reactivity Studies of Some Iridium (I) Complexes

IP4  M. D'Alpaos  GC/MS in Aroma Chemistry: A Comparison of Essential Oils and Flavours Extracted by Classic and Supercritical Techniques

IP5  M. D'Alpaos  MALDI/MS for the Evaluation of γ-Globulins Glycation Levels


IP7  V. Kováčik  Fragmentation of Per-O-methylated Oligosaccharides, Containing 2-N-acetamido-D-glucopyranose Unit under the Conditions of MIKE and CID FAB Tandem Mass Spectrometry

IP8  V. Kováčik  Structure Characterisation of Oligosaccharides, Containing 2-N-acetamido-D-glucopyranose unit using Metastable and Collision-Induced FAB Tandem Mass Spectrometry

IP9  V. Kováčik  Linkage Characterisation of Alditol Oligosaccharides by Fast Atom Bombardment Collision Induced Dissociation Tandem Mass Spectrometry of Sodium Cationized Ions

IP10  M. Olsthoorn  Structural Analysis of Temperature-Regulated Rhizobal Lipo-Chitin Oligosaccharides Using Mass Spectrometry

IP11  M. G. Santana-Marques  Discrimination Effects and Sensitivity Variations in MALDI Sample Preparation

IP12  P. Mauri  Analytical Strategies in the Structural Characterisation of Elcatonin by LC-DAD-ESI
IP13  P. Mauri  Mass Spectrometry Analysis of Flavonoids
IP14  V. Havlíček  Amino Acid Analysis in Ergopeptines
IP15  W. Danikiewicz  Ortho-Effects in the EI-induced Fragmentation of N-Alkyl-o-Nitroanilines
IP16  E. Maccioni  Electron Impact Mass Spectrometry of some Neuroleptic Aminoalkyl Thiophene Cycloalkanones
IP17  J. Leško  GC-MS(MID) Analysis of Residues of some Fungicides in Wines
IP18  K. Ludányi  Application of Capillary Electrophoresis and MALDI-MS in Oligonucleotide Research
IP19  L. Drahos  Thermal Energy Distribution of Peptides
IP20  V. Pátoprstý  Transglycosylation reactions of some glycosylamines
IP21  V. Pátoprstý  EI, FAB and CI MS in the Structure Elucidation of N-acetyl-glycosylamines and N-acetyldiglycosylamines
IP22  Š. Matejčík  Observation of the Nucleophytic Displacement (SN₂) Reaction Induced by Dissociative Electron Attachment in Binary Van der Waals Clusters
IP23  M. Pavlík  Positive Corona Discharge in an Ambient Air: Source of H⁺.(H₂O)ₙ Clusters
IP24  T. D. Märk  Electron Attachment Studies at High Energy Resolution to Molecules and Clusters of Atmospheric Relevance
IP25  J. Slobodnik  Degradation Studies of Environmental Pollutants in Water by On-line Solid-Phase Extraction and Liquid Chromatography/Particle Beam-Mass Spectrometry
IP26  V. Kardos  Advances Method for the Determination of Residues of Some Tranquilizers and Carazolol (Beta-receptor Agonizer) as Illegal Growth Promoters via GC/MS System from Edible Tissues of Animal Origin
IP27  T. Gál  Formation Mechanism of Polyatomic Species in Vacuum Discharge Plasma as Revealed by Isotope Tracers

19:30  Dinner
Wednesday, May 14, 1997

7:30  Breakfast

Chairman: K. Pihlaja

L15 8:00 - 8:45  
A. Harrison  
Chemical Ionization Mass Spectrometry: Analytical Applications of Ion/Molecule Reactions

L16 8:45 - 9:30  
J. Jalonen  
Adducts in Chemical Ionization Mass Spectrometry; Useful Species or Nuisance?

L17 9:30 - 9:50  
V. Pâtoprstý  
Pyridine - an Useful Reagent in Chemical Ionization Mass Spectrometry of Carbohydrate Derivatives

L18 10:10 - 10:30  
H.-Fr. Grützmacher  
Gas Phase Protonation of Aliphatic Amides and Diamides: Structures, Conformations and Proton-Bound Clusters

L19 10:30 - 10:50  
V. Kováčik  
Liquid Secondary Ion and Fast Atom Bombardment Mass Spectrometry of Methyl Glycosides Using Matrices Containing Carboxamides

L20 10:50 - 11:10  
W. Lindinger  
On-line Monitoring of VOC at ppt Levels by Proton Transfer Reaction Mass Spectrometry (PTR-MS)

L21 11:10 - 11:30  
J. Slobodník  
Various Approaches to Multiresidue Trace-Level Analysis of Environmental Pollutants by Automated Methods of LC/MS and LC/MS/MS

12:00  Lunch
Excursion afternoon

Buses leaving from Smolenice castle at 1:00 p.m.

The excursion will include:

1) Tour of the Červený Kameň Castle. 
Exposition of the medieval furniture and equipment, the picture gallery.

2) Visit to the exposition of the folk pottery and ceramics in Modra. 
Video demonstration of the pottery manufacturing (in English). There will be a possibility to purchase the pottery products.

3) Tour of the historical castle in Pezinok - 6:00 p.m. 
Gala-dinner in the Pezinok Castle - 6:30 p.m.

The departure of the buses to Smolenice is planned for 9:30 p.m., anticipated return at 10:00 p.m.
<table>
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<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>Title</th>
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<tr>
<td>8:00</td>
<td>Breakfast</td>
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<td></td>
<td><strong>Chairman: H.-Fr. Grützmacher</strong></td>
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<tr>
<td>L22</td>
<td>9:00 - 9:45</td>
<td>N. M. M. Nibbering</td>
<td>Chemical Research with the Use of Mass Spectrometry</td>
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<td>L23</td>
<td>9:45 - 10:30</td>
<td>M. Claeys</td>
<td>New Insights in Collision Induced Charge-Remote and Charge-Proximate Fragmentation in Saturated and Unsaturated Fatty Acids Derivatives.</td>
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<tr>
<td>12:35</td>
<td>Lunch</td>
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**Chairman: L. Cornides**

L28 14:00 - 14:45  
**K. Varmuza**  
Support of Systematic Structure  
Elucidation by Mass Spectral Classifiers and  
Exhaustive Isomer Generation

L29 14:45 - 15:30  
**A. Nikiforov**  
Computer Assisted Interpretation and  
Comparison of (LR) and (HR) GC-MS Data

L30 15:50 - 16:10  
**P. Vainiotalo**  
Characterisation of Small Molecular Weight  
Polyesters with MALDI/TOF Mass Spectrometry

L31 16:10 - 16:30  
**E. De Pauw**  
Electrospray Mass Spectrometry Study of  
Selective Macrotricyclic Dicarboxylates Inclusion  
Complexes

16:30 - 17:15  
**Poster Session II - Oral presentation**

17:15 - 19:00  
**Poster Session II**

II P1  
**D. Favretto**  
Ion Trap HPLC/ESI-MS in the Characterization of  
(Methoxymethyl)Melamine Resins

II P2  
**D. Favretto**  
Mass Spectrometry as Ancillary Tool in MOCVD  
Studies

II P3  
**E. De Pauw**  
Minimum Informations Required for Fast Medium  
Size Peptides (1-2kDa) Sequencing Using ESI/MS-MS

II P4  
**P. Traldi**  
Electrospray MS in Organometallic Chemistry.  
1. The Case of [Pt(η⁴-allyl)XP(C₆H₅)₃] Complexes

II P5  
**D. Kuck**  
Isomerization and Fragmentation of Long-lived  
Protonated Alkylcycloheptatrienes
II P6  R. Seraglia  Cosmetic Products Analysis: GC/MS and FAB/MS as Complementary Tools for the Characterization of the Ingredients of Mascara and Hair Dyes

II P7  V. Kubelka  Quantification of PAH in the Grilled and Smoked Meat

II P8  A. Raffaelli  Solid Phase Micro Extraction (SPME) Coupled with Ionspray and APCI LC-MS

II P9  A. Dobó  Determination of Muscat-Type Aroma Additives for Wines Using SPME Head-Space Sampling and GC-MS Analysis

II P10  M. Claeys  Characterization of Intermediate Products Formed During Cyanogen Bromide Cleavage of Peptides and Proteins by Electrospray Tandem Mass Spectrometry

II P11  M. D'Alpaos  FAB Mass Spectrometry of Some Macro cyclic Schiff Bases and Related Reduced Derivatives

II P12  G. Diamantini  Correlation of the Antimetastatic Properties of Aryltriazenes with their Electron Impact Ionization Mass Spectrometry

II P13  P. Biely  Identification of O-acetyl-O-trimethylsilyl Derivatives of Methyl -β-D-xylopyranoside and -glucopyranoside by EI MS

II P14  V. Kováčik  Negative-Ion Mass Spectra of Molybdate (VI) Complexes of D-Lyxose and D-Mannitol

II P15  O. Šimo  Mass Spectrometric Study Fragmentation of 8-Azaxantine Derivatives

II P16  M. V. Kosevich  Alcohol Cluster Formation Under Low Temperature SIMS/FAB Conditions

II P17  L. K. Galetich  Energy of Formation of Stacking Dimers of Pyrimidine as Revealed by Temperature Dependent Field Ionization Mass Spectrometry
II P18 S. Musil   Determination of Elemental Composition by Statistical Analysis of GC/MS

II P19 S. Gelosi   Role of SIMS in Brazing of Precious Alloys Analysis

II P20 C. Paradisi   Abatement of VOCs by Corona Discharge. A Study of the Reactivity of Trichloroethylene (TCE) under Atmospheric Pressure Ionization Conditions

II P21 W. Lindinger   Energy Dependence of the Isomerization of HCN$^+$ to CNH$^+$ via Ion Molecule Reactions

II P22 R. Seraglia   Structural Characterization of Highly Degraded Oligomer Component in Synthetic Tyrosine and Dopa Melanins by MALDI/MS

II P23 R. Seraglia   A Mass Spectrometry Study on Some 2-Bromopropanilides

II P24 R. Maffei Facino Characterization of Phenolic Constituents of Krameria Triandra Roots with Antimicrobial/Radical Scavenging Activity by LC-MS and FAB-MS/MS

II P25 G. Pócsfalvi   Microheterogeneity Characterization of a Trichorzianine-A Mixture from Trichoderma Harzianum

II P26 S. Gelosi   Electroformed Objects for Jewelry: Surface and Near-Surface Analysis by SIMS

II P27 V. Pátoprstý   Studies on Composition of Lipopolysaccharides from Coxiella Burnetii

19:00 Farewell Dinner accompanied by the performance of the folk dance group
Friday, May 16, 1997

8:00 Breakfast

Chairman: W. Lindinger

L32 9:00 - 9:45 K. Vékey
Characterisation of Wine Aroma Compounds Using Solid Phase Microextraction (SPME) GC-MS

L33 9:45 - 10:05 T. D. Märk
Low Energy Collisions of Polyatomic Ions and Dimer Ions with a Solid Surface

L34 10:05 - 10:25 I. Cornides
Carbon Clusters with Metallic Heteroatoms - the Access to Metallofullerenes?

L35 10:45 - 11:05 S. Matt
Electron Induced Ionization and Dissociation of Fullerene Ions

L36 11:05 - 11:25 O. Kóréh
Study of the Decomposition of Sulphur Hexafluoride Gas by Gas Chromatography/Mass Spectrometry

12:00 Lunch

13:00 Departure of the buses to Bratislava