I. STAFF
Full Professors:
Dušan Bustin PhD, DSc; Ján Krupčík, PhD, DSc, Jozef Lehotay, PhD, DSc, Ján Mocák, PhD, DSc
Associate Professors:
Ernest Beinrohr, PhD, Eva Brandšteterová, PhD, Miroslav Čakrt, PhD, Ján Labuda, PhD, Eva Matisová, PhD, DSc, Drahomír Oktavec, PhD, Miroslav Rievaj, PhD, Jozef Polonský, PhD, Viktor Vrábel, PhD
Assistant Professors:
Eva Benická, PhD, Tatiana Buzínaiová, PhD, Andrea Hercegová, Elena Korgová, PhD, Jarmila Laštínková, Pavol Májek, PhD, Alena Manová, PhD, Pavol Tarapčík, PhD, Mária Vaničková, PhD
Reader:
RNDr. Magdaléna Valachovičová
Research Fellows:
Miriam Bučková, PhD, Ján Dzurov, Adriana Feťcová, PhD, Katarína Hroboňová, PhD, Pavol Kubalec, PhD, Jana Sádecká, PhD, Ivan Skačání, PhD, Ivan Španík, PhD, Peter Tomčík, PhD
PhD Students:
Branko Balla, Alica Čaniová, Jana Ďungelová, Peter Korytár, Petra Kotianová
Technical staff:
Ladislav Bartalos, Danuša Bartalosová, Marta Benešová, Zuzana Cifrová, Ing. Jana Otrubová

II. TEACHING AND RESEARCH LABORATORIES
Laboratory of capillary gas chromatography
Laboratory of high performance liquid chromatography
Laboratory of electroanalytical methods
Laboratory of molecular spectrometry
Clean laboratory for trace analysis with atomic spectrometry (AAS, OES-ICP)
Laboratory of organic elemental analysis
Laboratory of organic synthesis
Laboratory of fluorescence analysis
Laboratory of capillary isotachophoresis
Laboratory of electrochemical pre-concentration for atomic spectroscopy
Laboratory of chemometry
Laboratory of bioanalytical chemistry

III. TEACHING

A. Undergraduate Study

4th semester
Analytical Chemistry I. (2-2 h) Krupčík, Labuda, Polonský, Vrábel
Laboratory Practice AC I. (0-4 h) Valachovičová

5th semester
Analytical Chemistry II. (2-2 h) Bustin, Čakrt, Lehotay, Polonský
Laboratory Practice AC II. (0-4 h) Korgová
Testing and Quality Control (1-1 h) Čakrt

6th semester
Semesters Project

7th semester
Atomic Spectrometry (2-0 h) Beinrohr
Anal.Chem.of Complex Inorg. Mixtures (2-0 h) Oktavec
Anal.Chem. of Complex Org. and Biological Mixtures (2-0 h) Brandšteterová
Lab.Practice I. (0-10 h) Matisová
V. CURRENT RESEARCH PROJECTS

A. Development and Application of Direct Injection Assays for HPLC Analysis of Some Drugs and Toxic Compounds in Biological Samples (Eva Brandšteterová)
The aim of the project is the development and application of new automated assays with the possibility of direct injection of biological samples into the HPLC system. New sorbents, especially with restricted access for macromolecules (Restricted Access Materials- RAM) and high retention and preconcentration ability for analyzed compounds are tested for the preseparation step. RAM precolumns with the recommended material have been integrated directly into the HPLC system what improves validation parameter values and minimizes the personal contact with biofluids. Direct sample injection of biological samples (hemolyzed blood, plasma, serum, urine, homogenates of tissue, supernatants of cell cultures, extracts of plants and milk) with the application of RAM materials has not been widely applied till now and the study of optimal extraction and retention conditions, interactions of analytes and matrix biopolymers with the sorbent enable to integrate the RAM extraction precolumn into the HPLC equipment.
The results obtained during the project research works:
- Some new assays have been developed for the direct achiral and chiral HPLC analysis of chosen drugs and their metabolites with the applications of various new sorbents in preseparation columns integrated on-line into the HPLC system and results have been compared with techniques, commonly used in biological sample handling. Column-switching system was applied for the development of new procedures in drug monitoring in clinical material and the HPLC analysis of biological compounds in food and plant samples.
- RAM sorbents have been chosen with acceptable hydrophobic behaviour for the analyzed compounds and elution parameters have been determined with the aim to achieve the sufficient preconcentration of analytes in biological matrices.
- The results of HPLC and electromigration methods (CE) have been compared for chiral separation of some drugs and their metabolites in clinical samples and some new methods have also been developed for direct ITP analysis of the group of drugs in biological material and organic acids in food samples. The study of interactions with the influence on selectivity of chiral drug separation has been realized, the possible steric influence, the effect of separated molecules caused by mobile and stationary phases have been studied and the separation mechanism for applied chromatographic system has been explained.

B. New Electroanalytical and Spectroscopic Systems for Ultra-trace and Speciation Analysis with Special Emphasis to Environmental and Clinical Problems. Optimization of analytical procedures (Dušan Bustin)
The aim of the project is the development of analytical methods for trace and ultratrace analysis of complex clinical and environmental samples. The results achieved during recent stage of research can be summarized as follows:
- Analytical methods for determination of Se and dithiocarbamates in environmental samples were developed and characterized metrologically. The methods apply Interdigitated Microelectrode Array in dual polarization mode.
- Metrological characterization and validation was accomplished for AAS determination of As and Se using electrochemical generation of corresponding hydrides.
- Analytical method for simultaneous determination of Zn, Cd, Pb and Cu using flow galvanostatic stripping coulometry was developed.
- A new method for determination of electroactive species using total electrolysis inside porous electrode was developed. The method was tested for determination of some metals (Fe, Cr) and non-metals (halogenides, oxygen, nitrates, organic species) in aquatic samples.
- A new method of determination of limit of detection was applied in different regions of trace analysis.
- Interfering signals in voltammetry were deconvoluted using their transformation by semidifferentiation.

C. Trace analysis of selected analytites in complex organic systems by combination of preconcentration techniques and capillary gas chromatography (Eva Matisová)
The project is oriented to the development of methods for the trace analysis of selected, particularly volatile and semivolatile compounds in complex organic systems - in environmental matrix (predominantly water) utilising preconcentration techniques in combination with capillary GC. A part of the project is devoted to the miniaturisation in analytical chemistry - to the development of microextraction methods for the sample preparation, large volume injection (small sample size necessary) in capillary GC. A part of the project is connected with the development of high speed GC and combination with preconcentration techniques for the analysis of semivolatiles polarity thermolabile compounds. High speed gas chromatography allows the shortening of the time of analysis have evaluated the present state of the theory of high speed capillary GC, fa. influencing the speed of analysis and instrumentation which could be utilitzed for GC – conventional and ultra high speed GC utilising specially development Instrumentation. For the aims of trace analysis we have used high speed GC with own column injection. We have shown the necessity of the combination of conventional dimensions precolumn with the narrow bore analytical capillary column, which allows a sample introduction without the peaks broadening. The influence of experimental parameters, as column head pressure, injection volume, initiation temperature of the temperature programme and temperature gradient on peaks focusing was searched.

D. CEEPUS Project PL-0110-00/01 (Ján Mocák)
The Project, planned for the schoolyear 2000/2001, concerns 5 cooperating Universities: (1) Faculty of Material Science and Ceramics, University of Mining and Metallurgy, Kraków, Poland, (2) Institute für Analytische Chemie, Karl-Franzens-Universität, Graz, Austria, (3) Faculty of Chemistry & Chemical Technology, University of Ljubljana, Slovenia, (4) Department of Analytical Chemistry, Slovak University of Technology, Bratislava, Slovak Republic, and Institute of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Czech Republic.
The collaboration is focussed on education and research in analytical chemistry, especially at the postgraduate and graduate level, mainly in the following areas: development and improvement of contemporary analytical methods and procedures, monitoring the environmental pollution, application of the quality systems and accreditation requirements to the research and routine analytical laboratories. The following key activities have been planned for the Project:
1) Mobility of the PhD and Master degree students to improve their educational level and language skills.
2) Mobility of the teaching staff to increase their teaching performance.
3) Utilization of unique or rarely available instruments and experience of their operation by the cooperating partners - the students as well as academic staff.
4) Preparation of joint scientific outputs.

E. Development of new analytical methods in environment and pharmaceutical drugs in biological systems (Drahomír Oktavec)
1. The aim of this Project is:
   a) to develop methods for the determination of trace and ultra trace amounts of chosen toxic elements and compounds in the air, soils and waste products of industrial factories which would also allow to monitor their transition into the food chain of mammals,
   b) on the base of chromatographic methods to model conditions in biological materials and develop methods both for the determination of pharmaceutical drugs and their degradation products in biological systems as well as for the separation of enantiomers of pharmacologically active compounds,
   c) to study crystal and molecular structure of biologically active compounds by X-ray structure methods, which results are obliged as qualitative criteria for drugs.
2. In the frame of the project the very good results were achieved in the field of the study of some drugs by HPLC and structuraal analysis. Also, the som pollutants in environmental were studied. The students were inclued in the study and so the project had the very good education efficiency (diploma and projekt works). Some results of the study were used into education process in the field of practical student training. Besides of diplom and project works 7 lectures were presented on the international symposia and local conferences.
F. The development of modern method for teaching analytical chemistry supported by PC (Pavol Tarapčík)

This project is directed to overcome drawbacks of traditional teaching method by applying relatively individual work methods in front of PC in the field of analytical chemistry. Chemical equilibria as applied in analytical chemistry represents for students relatively complex problem both in chemical and mathematical description. The last one is often crucial in the classroom work but represents only the tool, not the content analytical chemistry. The principal aim of the project is: by minimising time consuming calculation in classroom open new possibilities to recognise chemical principles of analytical methods.

The main goals of this project are:
- to make simulating software for various analytical methods, mainly in the area of chemical equilibria in analytical chemistry,
- to make teaching procedures supported by simulating software, combining work methods in whole group by traditional method and in small groups (two-three students) with PC,
- to make templates for solving typical problems of analytical chemistry.

We have prepared new teaching software supports based on spreadsheet „EXCEL“. These products include:
software intended to assist teaching acid-base equilibria,
application software of chemical equilibria in analytical methods,
solved templates of typical analytical and equilibrium problems (on PC)
The textbook containing typical solutions of analytical problems was prepared as well.

V. COOPERATION
A. Cooperation in Slovakia
Department of Analytical Chemistry PrF UK Bratislava
Faculty of Natural Sciences, Comenius University, Bratislava
Faculty of Medicine, Comenius University, Bratislava
Faculty of Pharmacy, Comenius University, Bratislava
Food Research Institute, Bratislava
Institute of Veterinary Hygiene and Ecology, Trnava
National Institute of Oncology, Bratislava
Slovak Academy of Sciences, Bratislava

B. International Cooperation
Department of Analytical Chemistry, Palacky University, Czech Republic
Department of Chemistry, Gilman Hall, Iowa State University, Ames, IA 50011-3111, USA
Chiral separation of optical active compounds by GC and SFC
Department of Organic Chemistry, Gent University, Gent, Belgium
Chiral separation of optical active compounds by GC and SFC
Department of Oncology, University of California, San Diego, U. S. A.
Department of Pharmacology, McGill University, Montreal, Canada
Faculty of Material Science and Ceramics, University of Mining and Metallurgy, Kraków, Poland
Electrochemical trace analysis
Advanced chemometric evaluation of analytical data
Institute of Analytical Chemistry, University of Leipzig, Germany
Electrochemical methods in atomic spectroscopy
Institute of Pharmaceutical Chemistry, University of Muenster, Germany
Institute of Pharmacy, University of Liege, Belgium
National Research Institute of Health Science, Tokyo, Japan
Organic Compounds in Aerosols
Technical University Vienna, Institute of Analytical Chemistry, Vienna, Austria
Utilization of Capillary GC in Combination with reconcentration Techniques for the Analysis
C. Membership in Domestic Organizations and Societies
Editorial Board of the Slovak scientific journal Laboratory Diagnosis (J. Mocák)
Slovak Chemical Society at Academy of Science, Group of Analytical Chemistry (J. Krupčík)
Slovak Chemical Society, Chromatographic group (E. Brandšteterová)
Slovak Chemical Society, Bratislava (J. Labuda)
Slovak Research Technical Society (E. Brandšteterová)
Slovak Society of Industrial Chemistry, Bratislava (J. Labuda, M. Bučková, M. Vaničková)
Slovak Spectroscopic Society Bratislava (E. Beinrohr, A. Manová, J. Lašťincová)
D. Membership in International Organisations and Societies

Advisory board member of the Fresenius Journal of Analytical Chemistry (E. Beinrohr)
Federation of European Chemical Societies- delegate of the Slovak Chemical Society in the Division of Analytical Chemistry (J. Labuda)
Gesselschaft Deutscher Chemiker, Frankfurt (E. Beinrohr)
International Union Against Cancer, Switzerland (E. Brandšteterová)

E. Tempus Programme:

F. International Scientific Programmes:


2. SLOVAK – US UNIVERSITIES CO-OPERATION Project Title: Mechanistic study of chiral recognition in HPLC and HRGC, J. Krupčík
   The main objective of the project is to study some mechanistic aspects of chiral recognition in the direct separation of enantiomers by HPLC and HRGC. The project consists of following parts:
   1. An influence of structure and polarity differences in substituents bonded to the asymmetric carbon atom in enantiomers, and selectivity of a chiral selector in HPLC and HRGC shall be studied in detail. Modified $\alpha$-, $\beta$- and $\gamma$-cyclodextrins and macrocyclic antibiotics shall be used in gas and/or liquid chromatography as chiral selectors.
   2. Thermodynamic data which characterize overall and enantioselective interactions of the enantiomers with chiral selectors shall be collected to gain more insight into the mechanistic aspects of enantioseparation on modified cyclodextrins.
   3. A dependence of selectivity of a chiral column on the concentration of a chiral selector in polysiloxane solvent (a column coated with a mixed chiral phase and achiral phases) shall be compared with the overall selectivity of two columns coupled in series. In the column series, stationary phases in the individual chiral and achiral columns shall be identical with those used in column coated with the mixed chiral and polysiloxane phases.
   4. Reasons responsible for the temperature dependence of retention order shall be studied by the GC separation of enantiomers on modified $\alpha$-, $\beta$- and $\gamma$-cyclodextrins.
   5. For mechanistic studies of enantiomers separated by chiral HPLC on macrocyclic antibiotics indirect detection techniques shall be introduced.
   6. Selectivity of two chiral columns coupled in series for the direct separation of enantiomers by HRGC and RP HPLC shall be tuned by the change of mobile phase flow rate in individual columns. Elaborated optimum separation system shall be used for two dimensional separation of optically active compounds in natural samples.

Slovak Principal Investigator: Prof. Ján Krupčík, PhD. DSc., Department of Analytical Chemistry, CHTF STU in Bratislava, Slovak Republic
Main American Investigator: Prof. Daniel W. Armstrong, Department of Chemistry, Gilman Hall, Iowa State University, Ames, IA 50011-3111, USA


G. Visitors from Abroad

Prof. H. J. Vander Linde Pretoria, South Africa, March 1999 (1 day)
Profesor Jose Antonio Garcia Dominguez Institute of Physical Chemistry Rocosolano v Madrid, Spain (2 days)

H. Visits of Staff Members and Postgraduate Students in Foreign Institutions

B. Balla Graz, Austria, July 2-7 2000 (4 days)

E. Beinrohr Bonn, Deutchland, conference, June 12-16 2000 (5 days)
E. Beinrohr Bologna, Poland, June 19-21 2000 (3 days)
E. Beinrohr Warsaw, Poland, conference, June 26-30 2000 (5days)
E. Beinrohr Klivice, Poland, conference, July 9-13 2000 (5 days)
E. Beinrohr USA, conference, August 2-15 2000 (14 days)
VI. THESES AND DISSERTATIONS

A. Graduate Theses (MS Degree) for state examinations after five years of study in Analytical Chemistry (Supervisors are written in brackets)

Árendárková S.: In-electrode coulometric titrations (E. Beinrohr)

Bajdichová M.: Calculation of enantiomerization energy barrier of thermal labile optical active compound separated by gas chromatography on chiral phases (J. Krupčík)

Bendzárková I.: The determination of sorbic acid in food products (T. Buzinkaiová)

Ďungelová J.: Separations of some enantiomers of phenylcarbanic derivates by HPLC (J. Lehotay)
Fedorčáková A.: Speciation of phosphate salts in aqueous solutions (P. Tarapčík)
Fuknová M.: Analysis with DNA biosensor (J. Labuda)
Heilerová L.: Ninhydrin as a luminescence reagent (M. Čakrt)
Husáková G.: Electrochemical generation of hydrides for atomic spectroscopy (A. Manová)
Javorová S.: The study of Possibilities of RAM sorbents in HPLC of clinical sorbents (E. Brandšteterová)
Kotianová P.: Capillary gas chromatography and its utilisation in the analysis of mixtures of organic compounds (E. Matisová)
Mičič S.: Creation and adaption of Chemometrically and metrologically oriented Software (J. Mocák)
Nyúlová K.: Study of Spectral Properties and Separation of some Toxic Metal Ditiocarbamates (D. Oktavec)
Orošová K.: Isotachophoretic study of some drugs. (J. Sádecká)
Podhradská I.: HPLC analysis of phenolic acids in Melissa officinalis (E. Brandštetrová)
Rosincová D.: Determination of drugs using electrode modified with β-cyclodextrin (E. Korgová)
Vývleková Z.: Application of voltammetric microelectrodes in ultratrace analysis (M. Rievaj)
Zajíčková Z.: Use of gas chromatography and derivatization in analysis of selected compounds from environmental matrices (E. Benická)

B. Dissertations (PhD.):
Špánik I.: The study of mechanistic aspects of chiral separation in capillary gas chromatography on cyclodextrin stationary phases (J. Krupčík)

VII. Publications
A. Journals (* registered in Current Contents)
[17] Kohútěková V., Hrabáková L., Beinrohr E.: Význam pasívneho absorbolového plechov, zloženie pasivačnej vrstvy a možnosti jej hodnotenia. The importance of passivation of steel sheets, the


B. Conferences (* international conferences)


[5]* Beinrohr E.: Flow-through coulometry in the determination of trace, minor and major components. Book of abstracts 8th International conference on flow analysis, University of Warsaw, Poland, June 25. – 29. 2000, p. 48 - 48


[90]* Mátisová E.: Mikroextrakcia tuhou fázou a membránová extrakcia. Solid Phase Microextraction and membrane exparation (in Slovak). High speed gas chromatography and Preconcentration techniques, Millennium school, Department of analytical chemistry, Faculty of chemical technology, STU, Bratislava, Slovak republic, May 30. – 2. June 2000, p. 51 - 60

[91]* Mátisová E.: Štúdium interakcií pri separácii enantiomérov metódou HPLC. Interaction study of separation of enantiomers by HPLC (in Slovak). Sjezd České farmaceutické společnosti a XVI. lékárnické dny, Hradec Králové, Czech Republic, Abstract of lectures and posters, October 2000, p. 10


Vrábel V., Oktavec D., Sivý J., Marchalín Š.: Kryštálová štruktúra a biologická aktivita 1,4 – dihydropyridinových derivátov. 8th Conference Present State and Perspectives of Analytical Chemistry in Practice, Bratislava, Slovak Republic, September 18. - 21. 2000, p. 139 - 140

C. Books and Textbooks


D. Patents

E. PC Programmes

[1] Beinrohr E., Tarapčík P.: ph2 - General pH calculation for sytems including up to nine acid-base compounds.


[4] Tarapčík P.: Set of solved analytical and chemical equilibria problems using the ECXEL spreadsheet