CHEMOMETRICS V

Brno, Czech Republic - August 29 - September 2, 1999

The International Chemometric Conference organized by the Masaryk University, Brno, the Czech Chemical Society, the Slovak Chemical Society, the Hungarian Chemical Society, the Austrian Chemical Society (Working Group Computers in Chemistry), and

International Group for Correlation Analysis in Chemistry
(An Associated Organization of the International Union of Pure and Applied Chemistry)
PROGRAMME

Monday 30.8.
9.00 - 9.15 opening
9.15 - 10.00 I1 (Shorter)
break
10.30 - 11.15 I2 (Katritzky)
11.15 - 12.00 I3 (Héberger)
lunch
14.00 - 14.45 I4 (Brickmann)
14.45 - 15.05 O1 (Madden)
15.05 - 15.25 O2 (Raczynska)
break
16.00 - 16.20 O3 (Takeuchi)
16.20 - 16.40 O4 (Hirota)
16.40 - 17.00 O5 (Hálóvá)
17.00 - 17.20 O6 (Waisser)
18.00 get-together party

Tuesday 31.8.
9.00 - 9.45 I5 (Mocák)
9.45 - 10.30 I6 (Pajeva)
break
11.00 - 11.20 O7 (Nadar)
11.20 - 11.40 O8 (Preisler 1)
11.40 - 12.00 O9 (Lamparczyk)
12.00 - 12.20 O10 (Cukrowski)
lunch
14.00 excursion
18.00 party in wine cellar

Plenary invited lectures

11 John Shorter: The Prehistory of the Hammett Equation
17 Ignacy Cukrowski: Chemometrics in Electroanalytical Chemistry. Artificial Neural Networks (ANN) in Metal Complexes by Polarography.
18 Jean-Marie Lehn: Supramolecular Chemistry Toward Programmed Chemical
Oral communications

01 John E. Madden, Paul R. Haddad, Josef Havel: Prediction of Retention Times in Anion Chromatography Using Artificial Neural Network.

02 Ewa D. Raczyńska: Tautomerism in Hydroxypyridines. Substituent and Solvation Effects in the Gas Phase.


09 H. Lamparczyk, A. Jankowski, P. K. Zarzycki: Application of Principal Component Analysis for Comparison of Subject Species Drug Pharmacokinetics.


12 R. Rajkó: Uncertainty of Concentration Predicted from Linear Calibration Using Least Squares and Robust Regression Methods.


15 Ewa Cukrowska, Libuše Trnková, Rene Kizek, Josef Havel: Quantitative Analysis of Adenine-Cytosine Mixtures Using Artificial Neural Networks in Linear Scan Voltammetry and Differential Pulse Polarography.


17 Eva Pribylova, Miroslav Holik: Determination of the Accurate Values of Rate Constants and Thermodynamic Parameters from NMR Spectra.


19 Josef Havel: Optimization in CE: Experimental Design and Artificial Neural Networks.
Posters


P4 Josef Havel, Ladislav Zezula, Marta Farková: Optimization Based on the Use of Experimental Design and Artificial Neural Networks (ANN).

P5 Ewa Cukrowska, Ignacy Cukrowski, Josef Havel: Artificial Neural Network for Quantitative Evaluation of Complex Polarographic Data.

P6 Ewa Cukrowska, Libuše Trnkova, Rene Kizek, Josef Havel: Artificial Neural Networks for Quantitative Analysis of Adenin-Cytosine Mixtures by UV-Vis Spectrophotometry.

P7 Josef Havel, Michael Breadmore, Miroslav Macka, Paul Haddad: Artificial Neural Network Optimization and Modelling in Capillary Micellar Electrochromatography.


P13 Knut Baumann, Peter D. Wentzell: Estimation of Intercept Terms in Maximum Likelihood Principal Component Analysis.


P17 Miloslav Suchánek, Prashant Bhave: Measurement Uncertainty of Mercury Determination in Biotic Matrices.


P21 K. Héberger, M. Görgényi: Principal Component Analysis of Kováts Indices for Oxo Compounds in Gas Chromatography.


P24 M. Macháček: Cosine Coefficients and the Norm of Vector in Evaluating Potential Drugs.


P30 Steffen Thomas, Erich Kleinpeter: AROSIM - An Incremental System to Estimate $^{13}$C NMR Spectra of Substituted Aromatic and Heteroaromatic Compounds.

P31 Miroslav Holík: Multivariate Regression with Substituent Shift Increments. V. para-Substituted Biphenyls, 2-Phenylfurans, and 6-Methyl-6-phenylfulvenes.

P32 Miroslav Holík, Vladimír Proks: Multivariate Regression with Substituent Shift Increments. VI. Shiff Bases of para-Substituted Anilines with Benzaldehydes and $\gamma$-Formylpyridines.


P34 I. V. Ekelchik: Mathematical Model for the Determination of Components of Redox Couple by the Method of Multiple Standard Additives.

P35 V. K. Mukhomorov: Information Approach to Quantitative Description of Biological Activity of Substrates.


