# Conference Programme

## Sunday, Aug 29 - Day 0

Arrival to Pardubice

Accomodation in hotel "Harmony" or University hostel

16.00 – 20.00 Registration in Harmony hotel reception

# Monday, Aug 30 - Day 1

07.00 - 09.00 Breakfest

08.00 – 10.00 Registration at the Conference Center

10.00 - 10.30 Opening

10.30 – 11.15 Plenary lecture

**Richard Brereton**: Applications of Pattern Recognition

11.15 – 11.45 Coffee break

11.45 – 12.30 Plenary lecture

Vincenzo Esposito Vinzi: PLS Generalised Linear Regression: Foundations and Recent Advances with Variable Selection and Validation Procedures

12.30 – 13.30 Lunch

13.30 - 14.30 Oral presentations

Chairman: Richard Brereton

David Milde: Teaching Chemometry and Good Laboratory Practice at Palacky University in Olomouc

Manuel Zarzo: Analysis of multiblock data sets to identify the key process variables in a batch

polymerisation

Liudmila Larina: The Analytical Signal Modelling for the Analysis Accuracy Increase at Some Model

Determination by Stripping Voltametry in Environmental Objects

14.30 – 15.00 Coffee break

15.00 - 16.00 Oral presentations

Chairman: Michael Tenenhaus

Walter Focke: Correlating Physical Property Data with Canonical Pade Approximants Simeone Zomer: Active Learning Support Vector Machines For Optimal Sample Selection

in Classification with Application in Mass Spectrometry

Afshin R. Khorrami: Determination of Caffeine in Blake Tea Leaves with FTIR Spectrometry Using

Chemometrics A Comparision Between MLR, PLS, CLS as Calibration Models

17.00 Welcome evening with excursion

## Tuesday, Aug 31 – Day 2

7.00 - 9.00 Breakfest

09.30 - 10.15 Plenary lecture

Michael Tenenhaus: PLS and Sensory Analysis

#### 10.15 - 11.15 Oral presentations

Chairman: Harald Martens

Manuel Zarzo: Consistency analysis for PLS with variable selection to diagnose a dehydration process

Manuel Zarzo: Analysis of dynamic gas sensor response using chemometric methods Richard Brereton: Statistical Use of Analytical Chemical Data in Court Cases

11.15 – 11.45 Coffee break

11.45 – 12.45 Oral presentations

Chairman: Vincenzo Esposito Vinzi

Walter Focke: A Wilson local composition model for the viscosity of liquid mixtures

**Zdeněk Wagner**: Robust Estimation of Particle Size Distribution of Atmospheric Aerosols by Gnostic Theory **Evelyn Archery**: Simultaneous Multicomponent Analysi of Cu, Ni, Fe and Co Using Partial Least Squares

12.45 – 13.45 Lunch

14.00 – 16.00 Poster presentations

15.40 Refreshment

17.00 Excursion with historical programme

### Wednesday, Sep 1 – Day 3

7.00 – 9.00 Breakfest

09.30 – 10.15 Plenary lecture

**Harald Martens**: Multivariate and Multiblock Chemometrics: A Culture for the "New Bioinformatics"?

10.20 – 10.05 Plenary lecture

**Johan Trygg**: Recent Developments in PLS Regression: OSC Filters, Pure Profile Estimation and Bi-directional (X-Y) Modeling

11.05 – 11.30 Coffee break

11.30 - 12.30 Oral presentations

Chairman: Milan Meloun

Hana Šormová: Statistics and its Application During the Analysisi of Optical Spectra; Uncertainties and

Measured Spectroscopy Data

Jiří Militký: Improved Uncertainty Prediction Strategy

Selvarajah Shankar Kumar: Wavelength Based Classification Technique

12.30 – 14.00 Lunch

14.00 - 15.00 Oral presentations

Chairman: Jiří Militký

Jaroslava Hálová: EA of Mstructure-Activity Data (QSAR) Using GUHA

Tomáš Syrový: Multivariate methods in chemometrics

Milan Meloun: Minimizing the Effects of Multicollinearity in the Polynomial Regression

15.00 – 15.30 Coffee break

15.30 Company presentations

17.00 Excursion with cultural programme

## Thursday, Sep 2 – Day 4

7.00 – 9.00 Breakfest

9.30 - 11.30 Oral presentations,

Sujatha Subramainan: Optical Spectrum Analysis

Nagwa Abo El-Maali: Simultaneous Voltammetric Chemometric Determination of the Anticancer Drugs:

Tarabine PFS, Adriplastina and Methotexate

Jiří Militký: Tutorial on Statistical Modelling

11.15 – 11.45 Refreshment

12.00 Excursion

15.00 Lunch

## Friday, Sep 3 – Day 5

Departure