

2004



# ChemStat

## 2<sup>nd</sup> Information Bulletin



**International Chemometrics Conference**

*The international meeting of chemometricians and statisticians  
in Czech Republic*

August 30 to September 2, 2004  
Pardubice, Czech Republic  
a satellite meeting of Compstat 2004

CHEMSTAT 2004 is organized by TriloByte Statistical Software, University of Pardubice, University of Liberec, Czech Chemical Society and its Chemometrics section. Proceedings published by John Wiley.



## International Chemometrics Conference

### 2<sup>nd</sup> Information Bulletin

*The international meeting of chemometricians and statisticians  
in Czech Republic*

This information booklet contains updated information of the conference organization, location, topics and time schedule. We hope that you will enjoy your stay at the conference. All registered participants will receive another update if necessary during August via e-mail.

### Preliminary programme

<p><b>Sunday, Aug 29 – Day 0</b> Arrival to Pardubice Accommodation in hotel „Harmony“ or University hostel 16.00 – 20.00 Registration in Harmony hotel reception</p>	
<p><b>Monday, Aug 30 – Day 1</b> 7.00 – 9.00 Breakfast in Harmony hotel 8.00 – 10.00 Registration at Conference Center 10.00 – 10.30 Opening 10.30 – 11.15 Plenary lecture 11.15 – 11.45 Coffee break 11.45 – 12.30 Plenary lecture 12.30 – 13.30 Lunch 13.30 – 14.30 Oral presentations 14.30 – 15.00 Coffee break 15.00 – 16.00 Oral presentations 17.00 Welcome evening with excursion</p>	<p><b>Tuesday, Aug 31 – Day 2</b> 7.00 – 9.00 Breakfast in Harmony hotel 09.30 – 10.15 Plenary lecture 10.15 – 11.15 Oral presentations 11.15 – 11.45 Coffee break 11.45 – 12.45 Oral presentations 12.45 – 13.45 Lunch 14.00 – 16.00 Poster presentations 15.40 Refreshment 17.00 Excursion with historical programme</p>
<p><b>Wednesday, Sep 1 – Day 3</b> 7.00 – 9.00 Breakfast in Harmony hotel 09.30 – 10.15 Plenary lecture 10.20 – 10.05 Plenary lecture 11.05 – 11.30 Coffee break 11.30 – 12.30 Oral presentations 12.30 – 14.00 Lunch 14.00 – 15.00 Oral presentations 15.00 – 15.30 Coffee break 15.30 Company presentations 17.00 Excursion with cultural programme</p>	<p><b>Thursday, Sep 2 – Day 4</b> 7.00 – 9.00 Breakfast in Harmony hotel 9.30 – 11.30 Oral presentations 11.15 – 11.45 Refreshment 12.00 Excursion 15.00 Lunch</p>
<p><b>Friday, Sep 3 – Day 5</b> Departure</p>	

*Tutorial lectures on regression, exploratory and multivariate statistical methods will be available for those interested alternatively in afternoons.*

## How to get there

Arrive at Prague International airport Ruzyně  
Take a taxi to the main Wilson Railway Station (ca 500 CZK) or a bus to Vitezne Namesti, then subway to the main Wilson Railway Station (longer, but cheaper). Take any express train to Pardubice (approx CZK 200, 90 minutes). Get off in Pardubice and take a trolley no. 3 or a bus no. 4 to Cihelna – University Campus (about 6 stops, you need to buy a ticket first – CZK 9). Exact location of the conference is 50°02'58.3" North, 15°45'58.7" East.

## Currency

czech crown (CZK)  
32 CZK = 1 Euro or 25 CZK = 1 USD  
(rates are approximate)

## Accommodation

Participants are accommodated in Harmony Hotel or guest apartments of Student hostel, according to their choice. Both places are within 5 minutes walking distance from the conference site. Coordinates: 50°02'50.9" North, 15°45'48.4" East.



Harmony hotel with breakfast, ca. 300m away from the conference site.



Student Hostel, breakfast served in the Harmony hotel, 100m away from the conference site.

## Conference site



All lectures are held in the University Conference center at Pardubice-Cihelna

### Scientific committee:

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## The Aim of the Conference

To contribute to the development of a strategy and techniques for European research in computerized analysis, utilizing and communicating chemical information.

To present current problems and solutions in technology and applied research.

To make industry aware of strategic research methods and results and help to put research in life.

To make advanced methodology used in academia applicable to industrial scale problems.

To seed statistical approaches, thinking and knowledge in industrial research.

## Selected accepted lectures

Outstanding papers from the proceedings will be re-published by J. Wiley in a special issue of Journal of Chemometrics in summer of 2005.



### *Invited plenary lectures authors (alphabetically):*

Richard Brereton, *University of Bristol, UK*, Harald Martens, *The Royal Veterinary and Agricultural University Denmark*, Michel Tenenhaus, *HEC Paris*, Johan Trygg, *Umea University, Sweden*, Vincenzo Esposito Vinzi, *Universita degli Studi di Napoli*

Surname	First name	Country	Paper Title
Nagwa	Abo El-Maali	Egypt	Simultaneous Voltammetric Chemometric Determination of the Anticancer Drugs: Tarabine PFS, Adriplastina and Methotexate
Evelyn	Archery	South Africa	Simultaneous Multicomponent Analysis of Cu, Ni, Fe and Co Using Partial Least Squares
Adegbola	Ayobami	Nigeria	Exploratory Data Analysis - Addressing the Context in which Chemometrics Works
Marek	Brabec	Czech Republic	State-Space Dynamic Model for Estimation of Radon Entry Rate, Based on Kalman Filtering
Richard	Brereton	United Kingdom	1:Applications of Pattern Recognition; 2:Statistical Use of Analytical Chemical Data in Court Cases
Walter	Focke	South Africa	1:Correlating Physical Property Data with Canonical Pade Approximants; 2:A Wilson Local Composition Model for the Viscosity of Liquid Mixtures
Jaroslava	Hálová	Czech Republic	EA of Structure-Activity Data (QSAR) using GUHA
Liudmila	Larina	Russia	The Analytical Signal Modelling for the Analysis Accuracy Increase at Some Model Determination by Stripping Voltametry in Environmental Objects
Harald	Martens	Denmark	Multivariate and Multiblock Chemometrics: A Culture for the "New Bioinformatics"?
David	Milde	Czech Republic	Teaching Chemometry and Good Laboratory Practice at Palacky University in Olomouc
Muili	Mubarak Akorede	Nigeria	Development of Chemometric Software
Afshin	R. Khorrami	Iran	Determination of Caffeine in Blake Tea Leaves with FTIR Spectrometry Using Chemometrics A Comparison Between MLR, PLS, CLS as Calibration Models
Gbadamosi	Ramoni Adewale	Nigeria	How to Design Software
Selvarajah	Shankar Kumar	India	Wavelength Based Classification Technique
Sujatha	Subramainan	India	Optical Spectrum Analysis
Hana	Šormová	Czech Republic	Statistics and its Application During the Analysis of Optical Spectra; Uncertainties and Measured Spectroscopy Data
Michel	Tenenhaus	France	PLS and Sensory Analysis
Johan	Trygg	Sweden	Recent Developments in PLS Regression: OSC Filters, Pure Profile Estimation and Bi-directional (X-Y) Modeling
Vincenzo Esposito	Vinzi	Italy	PLS Generalised Linear Regression: Foundations and Recent Advances with Variable Selection and Validation Procedures
Zdeněk	Wagner	Czech Republic	Robust Estimation of Particle Size Distribution of Atmospheric Aerosols by Gnostic Theory
Manuel	Zarzo Castello	Spain	O:Analysis of Multiblock Data Sets to Identify..., P1:Consistency Analysis for PLS with Variable Selection..., P2:Analysis of Dynamics for Sensor Response with...
Simeone	Zomer	United Kingdom	Active Learning Support Vector Machines For Optimal Subset Selection in Classification

### *Timeline for papers submitted for Journal of Chemometrics (J.Wiley).*

1. Submission of manuscripts: September 30, 2004
2. Return of peer-reviewed manuscripts to authors: 31 December 2004
3. Deadline for re-submission of revised articles: February 28, 2005
4. Publication for Early View on Wiley InterScience April/May 2005
5. Publication of Special Issue June 2005



## Conference topics

Statistical Molecular Design – PCA/PCR/PCL/SIMCA – Regression, Calibration – Generalisation of Linear Models – Soft and Classical Modelling – Simulation – Stochastic Methods – Multivariate Analysis – Robust Methods – Classification, Clustering – Applied Multivariate Methods – Optimization, Genetic Algorithms – Analysis of Spectroscopy Data – Exploratory Analysis of Multivariate Data – Neural networks applications – Graphing an imaging – Spatial Variability – Industrial Quality Control, SPC, QI, QA – Quality assurance in laboratory – Validation, accreditation – Free Software – Teaching chemometry – Exhibition and Poster Section.



## Conference Fees

*(see registration form for details)*

Regular conference fee €340

CompStat participants fee €150

(Members of ČSCH €260)

Student conference fee €150 (ISIC Card required)

Early payment before March 31 is reduced by 20%

Late payment after June 30 is raised by 10%

Hostel accommodation (breakfast not incl.) €90

Hotel accommodation (breakfast incl.) €220

Lunches €70

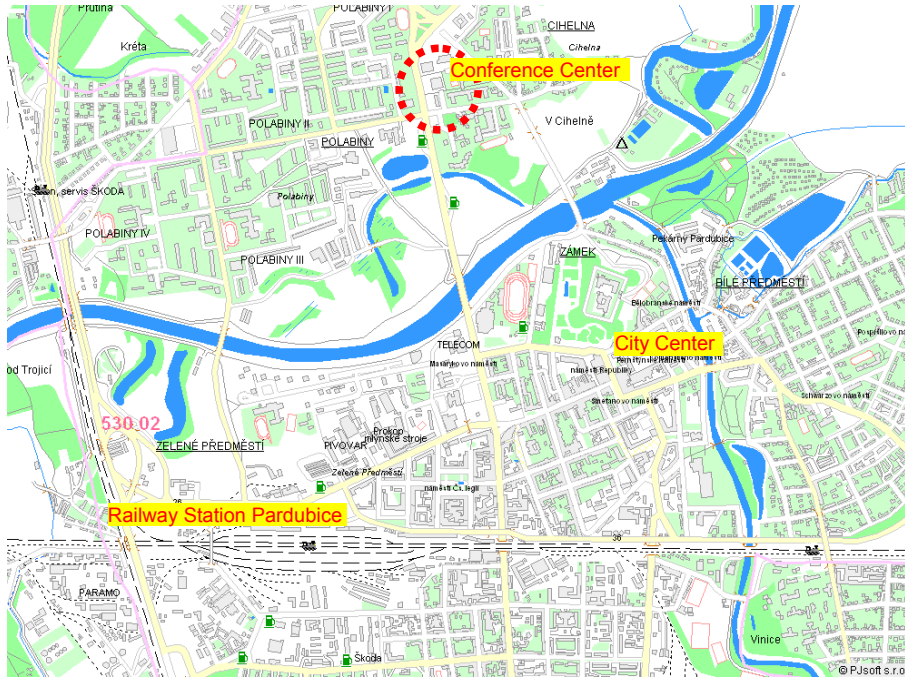
Party & Excursion €60



**Pardubice chateau**

## Pardubice - location, maps

Pardubice is a historical town (100 000 inhab.), ca 100 km east of Prague, easily accessible by train. Pardubice is a home of chemical industry (petrochemistry, polymers, inorganic, explosives). Chemstat conference is situated in a new conference facility at University of Pardubice.



Map 1 – Conference center and Pardubice city



Map 2 – Conference center and Accommodation



## Sponsors of the conference

We wish to thank sponsors of the conference:



University of Pardubice



Technical University of Liberec



Czech Chemical Society



TriloByte Statistical Software



Camo, The Unscrambler Software



For further information visit

[www.trilobyte.cz/chemometrics](http://www.trilobyte.cz/chemometrics)

We are looking forward to meet you in Pardubice, city of sports, gingerbread, beer and more.

*Organizers*

