



CAC-2004

9th International Conference in Chemometrics in Analytical Chemistry

New Challenges for a Maturing Science

September 20-23, 2004
Lisbon, Portugal

Lisbon, August 20th 2004

Dear CAC-2004 Participant

Please find below important information regarding your attendance of CAC-2004.

0. Pre-Conference Courses

1. Welcome Reception (Sun 19th)

2. CAC-2004 location

3. WIFI: wireless internet access

4. Poster & Paper Preparations

5. Awards: YCA & Best Poster Award

6. Social Program

7. Before or After CAC-2004: Extending your staying in Portugal

8. Hotel Reservations

9. Reaching your Hotel from the Airport

10. Late Registrations & Payments

11. CAC-2004 Schedule

CAC-2004 Secretariat

Centre for Biological & Chemical Engineering
IST, Av. Rovisco Pais, Lisbon 1049-001, Portugal

tel. (+351) 21 841 9838

fax: (+351) 21 841 9197

<http://dequim.ist.utl.pt/cac2004>

cac2004@ist.utl.pt

0. PRE-CONFERENCE COURSES

There are 6 one-day / half-day courses on the weekend 18 & 19 th of Sept. (9:00 AM to 5:00 PM). PRE-CONFERENCE COURSES are held at the Chemical Engineering Department at IST (South Tower - 5th floor).

A separate program will be sent to each of registered participants.

If you have not yet registered, don't miss the chance of taking one or more courses with some of the experts present at CAC-2004. We can still accept registrations. Go to the CAC-2004 web site and register separately for the course(s) of your choice. You may also enroll a pre-conference course on the day of the course if you can pay for it by cash or credit card at the secretariat.

1. WELCOME RECEPTION

Open to all CAC-2004 registered participants (with or without social program enrollment) and all accompanying persons that have registered in the Social Program.

Buses leave at 5:30 PM from and return by 10:30 PM to Holiday Inn Lisbon.

The Reception will include the Lisbon-Experience multimedia show by the River Tagus and a buffet dinner at AIP Restaurant (Junqueira) at which you will be able to collect the conference materials.

2. CAC-2004 LOCATION

CAC-2004 will be hosted at IST (Technical University of Lisbon) Congress Center. All IST's entrances will have indications on how to reach the Congress Center. As the Congress Center is just across the street from Holiday Inn Lisbon head for this Hotel and then follow the directions given there at the entrance.

3. WIFI

IST's Congress Center is served by a WIRELESS WWW access. You may thus bring your laptop/notebook with an adequate WIFI connection device and access your email and WWW during CAC-2004. This service will be free for all CAC-2004 participants.

You may also have internet access from your hotel lobby or hotel room. At least the recommended Hotels have both or one of them.

We'll try to arrange a couple of PC's so that people not having other means of checking their email, may do it during CAC-2004.

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4. ORAL & POSTER PRESENTATIONS, and PAPER Preparation / Submission

No distinction is made between oral and poster presentations as to their chance of getting published in the special volume of *Analytica Chimica Acta* containing selected contributions to CAC-2004.

- ORAL PRESENTATIONS are 25 or 40 min long.

Presenting AUTHORS must COMPLY with their assigned time leaving 3-5 min at the end of their presentations for clarifying questions from the audience.
- POSTER PRESENTATIONS will be scheduled as mentioned in the Scientific Program (text below and posted on the web site).

Posters must be no greater than 1,2 m (height) x 0.9 m (width).

Posters will be grouped into 2 groups, and each group will be on display on 3 poster sessions:

- posters belonging to themes 1, 4 and 6 will be on display on Monday (AM/PM) & Tuesday (AM)
- posters belonging to themes 2, 3 and 5 will be on display on Wednesday (AM/PM) & Thursday (AM)

To find out to which session your poster was assigned, please go to the authors list posted on CAC-2004's website
http://dequim.ist.utl.pt/cac2004/abstracts/authors_list.html

A best poster award will be given to the best CAC-2004 poster (see below #5).

POSTER AUTHORS MUST BE BY THEIR POSTERS during the POSTER SESSIONS.

POSTER authors are encouraged to bring several one-page printouts of their posters and hang those copies by their posters for distribution to interested participants.

PAPER SUBMISSION.

You must have received by now an email from ELSEVIER describing the paper on-line submission procedure. An ELSEVIER representative will be present at CAC-2004 in case you have any questions.

A Book of Abstracts will be distributed to all registered participants containing the supplied abstracts of all Oral & Poster presentations.

5. AWARDS

YCA. ELSEVIER sponsors every 2-years the Young Chemometrician Award. The nomination is coordinated by the *Chemometrics & Intelligent Laboratory Systems* Editorial Board and the award is presented during CAC meetings. The YCA will be presented during the Conference Banquet on Tuesday.

BPA. ELSEVIER will also sponsor the Best Poster Award at CAC-2004. This award will be given to the most voted by participants poster presented at CAC-2004. Each CAC-2004 participant has one ballot that should be cast until just after the 2nd poster session on Wednesday the 22nd. The award consists in one € 500 cheque and will be announced and given at the end of the day on Wednesday.

6. SOCIAL PROGRAM

The social activities during CAC-2004 include:

SUN 19th. Welcome reception (multimedia show by the Tagus & Buffet Dinner)

TUE 21st. Bus Tour (Cascais & Sintra) and Conference Banquet (Colares Wine Cellar)
Buses stop at CASCAIS cost line village (45 min) and SINTRA (2 h). You may visit points of interest (e.g., palaces or museums) at your own pace or simply sightseeing.

WED 22nd. Lisbon Oceanarium Visit
The participants will get to the Oceanarium by subway leaving just after the afternoon session, from the Congress Center. Dinner on your own after the visit, at Nations Park restaurant district.

With the exception of the Tuesday program, all other activities are open to all CAC-2004 registered participants (with or without social program enrollment) and all accompanying persons that have registered in the Social Program.

SOCIAL ACTIVITIES MEETING POINTS for CAC-2004 participants and accompanying persons:

SUN 19th – at 5:30 PM in front of Holiday Inn Lisbon returning at same point at 10:30 PM.

TUE 20th – at 2:00 PM in front of Holiday Inn Lisbon returning at same point at 11:30 PM.

WED 22nd – at 6:00 PM at the Congress Center. Return on your own (e.g., subway).

You may subscribe to the social package at CAC-2004 until Monday 20th but payment of the applicable fee must be made by cash or credit card.

7. BEFORE or AFTER CAC-2004: Extending your staying in Portugal

You can easily find on the WWW a variety of touristic sites about Lisbon and Portugal. You may download a small file prepared by the CAC-2004 Secretariat on some of the possible points of

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interest, at <http://dequim.ist.utl.pt/cac2004/Tourism.pdf>. Not included in that file, Algarve (beaches) and Azores & Madeira Islands are also very nice places to visit.

8. HOTEL RESERVATIONS & REDUCED AIR FARES

You should book your Hotel ASAP as we will have to let go CAC-2004's blocked rooms at selected Hotels, 2 weeks before CAC-2004. See the suggested list of budget hotels on CAC-2004 web site and mention CAC-2004 to book out of the blocked rooms.

TAP Air Portugal is granting CAC-2004 participants a 10% reduction on Economy tickets and 20% off in Executive Class. To benefit from this reduction you must buy the tickets on-line on their website. For more information on how to apply for the discount, send an email to Mrs Wendy Onofre (wonofre@tap.pt) or contact her or any other TAP representative directly at:
TAP Air Portugal - Marketing and Sales Support - Phone: +351 21 8416730 - Fax: +351 21 8416278

9. REACHING your HOTEL from the AIRPORT

The best way is by TAXI, but there is also a bus called Airport City Express.

A TAXI costs around 10-15 euros from the airport to the recommended hotels, plus 1.5 euro per piece of luggage store on the trunk. The ride takes 15-20 min (double this time during rush hour).

We strongly recommend that you PRE-PAY your taxi by buying a TAXI voucher at the airport arrivals terminal (the kiosk inside the terminal is clearly marked in English and other languages).

10. LATE REGISTRATIONS / LATE PAYMENTS

Make sure you have REGISTERED on the WEB SITE as all logistics starts from there (ID badges, lunch counts, tickets, buses, etc) and that you or your institution have paid your registration.

We may limit access to CAC-2004 premises to non-registered participants and to registered participants with non-paid registrations. WHEN in DOUBT about payment or for LATE PAYMENTS obtain from your institution and BRING WITH YOU a proof of payment of your CAC-2004 registration.

You may subscribe to the social package at CAC-2004 until Monday 20th but payment of the applicable fee must be made by cash or credit card. You may also enroll a pre-conference course on the day of the course if you can pay for it by cash or credit card at the secretariat.

11. CAC-2004 Schedule

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You may now download CAC-2004 schedule and Scientific Program from the Conference's web site.

For updated information on CAC-2004 please visit the web site <http://dequim.ist.utl.pt/cac2004>.

We hope you can enjoy your stay in Lisbon and make the most out of your CAC-2004 attendance both scientifically as well as a social experience.

We look forward to welcome you in Lisbon next September

Yours sincerely

Jose Cardoso de Menezes and Joaquim Esteves da Silva

CAC-2004
Organizing Committee

CAC-2004 Secretariat

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CAC-2004

Scientific and Social Program

Saturday & Sunday Sept. 18th & 19th

9:00 AM - 5:00 PM - PRE-CONFERENCE COURSES

Chemical Engineering Dept. IST (South Tower, 5th floor). Registered participants will receive a separate program.

SUNDAY, Sept 19th

5:30 PM WELCOME RECEPTION by the TAGUS RIVER

ALL INVITED including accompanying persons

Buses leave from Holiday Inn near IST, at 5:30 PM and return at 10:30 PM.

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Monday Sept. 20th

8:25 - 8:50 AM - Opening Ceremony

8:50 - 9:30 AM - Harald Martens
Chemometrics and the new "omics": Semi-soft modelling and interpretation

9:30 - 9:55 AM - Peter D. Wentzell
Chemometrics, Microarrays and the Secret Life of Yeast

9:55 - 10:20 AM - Peter B. Harrington
Chemometric Considerations in Proteomic Analyses of Bacteria by Mass Spectrometry

10:20 - 11:00 AM - Coffee-break -POSTER SESSIONS 1,4 & 6

11:00 - 11:40 AM - Age K. Smilde
Chemometric Challenges in Systems Biology

11:40 - 12:05 AM - Royston Goodacre
Explanatory analysis and optimisation of metabolomics and proteomics data via genetic search

12:05 - 12:30 AM - Javier Saurina
Quantification strategies in MCR-ALS. Focus on complex biological and clinical samples.

12:30 AM - 1:30 PM - LUNCH – BUFFET served at HOLIDAY INN LISBON

1:30 - 2:10 PM - Steven D. Brown
Novel Approaches to Classification for Use with High-Dimensional Data from Informatics and Metabolonomics.

2:10 - 2:35 PM - Modest Korff
Visualization of complex relationships between ligands and their biological targets by combining linear and non-linear mapping techniques.

2:35 - 3:00 PM - Beata Walczak
Automated matching of the two dimensional gel electrophoresis images.

3:00 - 3:40 PM - Coffee-break - POSTER SESSIONS 1,4 & 6

3:40 - 4:05 PM - Chris Watts
FDA's Process Analytical Technology (PAT) Initiative. Video conference from FDA in Washington DC.

4:05 - 4:30 PM - Vicki Loades
Applications of Chemical Imaging and Multivariate Image Analysis in the Pharmaceutical Industry.

4:30 - 4:55 PM - Anthony Walmsley
Can you hear it coming? – Early warning and tracking process changes in a fluidised bed using acoustics.

4:55 - 5:35 PM - Magni Martens
Chemometrics and Sensometrics in Analysis of Quality.

5:35 - 6:30 PM - Bernard Vandeginste (Moderator)
Special Session on The History, Foundations and The Founding Fathers of Chemometrics

EVENING FREE

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Tuesday Sept. 21th

8:25 - 9:05 AM - Svante Wold

The four levels of PAT (process analytical technology) and associated risks and benefits in pharmaceutical production.

9:05 - 9:30 AM - Marc Champagne

Using On-line Process Chemometrics Diagnostics to Improve the Product Quality

9:30 - 9:55 AM - Chengjian Xu

The use of Target Factor Analysis(TFA) for Studying Chemical Processes.

9:55 - 10:20 AM - Nouna Kettaneh

Multivariate Batch Monitoring and Fault Detection in Pharmaceutical Production.

10:20 - 11:00 AM - Coffee-break - POSTER SESSIONS 1,4 & 6

11:00 - 11:40 AM - Theodora Kourti

Abnormal Situation Detection utilizing Process Analytical Technology and Process Data - The state of the art in industry.

11:40 - 12:05 AM - Anders Björk

Monitoring Beating of Kraft Pulp Using Acoustic Measurements with a Standard PLS Model and a PCA-based Hierarchical Model.

12:05 - 12:30 AM - Michael J. Piovoso

Improved Process Understanding and Process Monitoring Via Chemometrics.

12:30 AM - 1:30 PM - LUNCH – BUFFET served at HOLIDAY INN LISBON

2:00 PM - SOCIAL PROGRAM

Registered participants in the Social Program

Buses leave from Holiday Inn near IST, at 2:00 PM and return at 11:30 PM.

AFTERNOON - Conference Tour to Cascais & Sintra World Heritage Village

EVENING - Conference Banquet at Colares Wine Cellar

Wednesday Sept. 22th

8:25 - 9:05 AM - Babatunde A. Ogunnaike
PRODUCT DESIGN AND OPTIMIZATION: An Emerging field with Challenges and Opportunities for Novel Data Analysis and Experimental Design Techniques

9:05 - 9:30 AM - Peter Zinn
Adaptive Chemistry: Product Development Applying Principles of Natural Evolution

9:30 - 9:55 AM - James M. Brown
Virtual Assays

9:55 - 10:20 AM - Elaine Martin
Sensor Data Fusion – The Sum of Two Halves is Greater Than the Whole

10:20 - 11:00 AM - Coffee-break - POSTER SESSIONS 2,3 & 5

11:00 - 11:40 AM - Romà Tauler
Resolution and Distribution of Main Contamination Sources in the Environment by Means of Bilinear and Trilinear Models and Methods

11:40 - 12:05 AM - Sylvie Roussel
Comparison of multivariate discrimination methods for GMO Detection based on near-infrared spectroscopic measurements

12:05 - 12:30 AM - Alisa Rudnitskaya
Multicomponent analysis of fermentation growth media by the Electronic Tongue

12:30 AM - 1:30 PM - LUNCH – BUFFET served at HOLIDAY INN LISBON

1:30 - 2:10 PM - Lutgarde Buydens
Chemical and Diagnostic Information from Magnetic Resonance Spectra and Images

2:10 - 2:35 PM - Sabine Van Huffel
On the equivalence between Total Least Squares and Maximum likelihood PCA with Applications in in-vivo Magnetic Resonance Spectroscopy Data Quantification

2:35 - 3:00 PM - Márcia M. C. Ferreira
Quantitative Analysis and Classification of AFM Images of Human Hair

3:00 - 3:40 PM - Coffee-break - POSTER SESSIONS 2,3 & 5

3:40 - 4:05 PM - Juergen von Frese
Microarray data analysis and its application to cancer diagnostics.

4:05 - 4:30 PM - Barry Wise
Classification of Cervical Tissue with Evoked Tissue Fluorescence Images Using 2- and 3-way Methods

4:30 - 4:55 PM - Sven Jacobsson
Peak alignment of NMR signals

4:55 - 5:35 PM - David Haaland
Multivariate Analysis of Hyperspectral Images for Biotechnology Applications.

**Wednesday Sept. 22th
(cont.)**

5:35 - 6:00 PM - Best Poster Awards

6:00 PM - LISBON OCEANARIUM

ALL INVITED including accompanying persons.

MEETING POINT at the CONGRESS CENTER at 6:00 PM

By METRO from IST station arriving at EXPO at 6:45 PM

Last entrance in the Oceanarium at 7:00 PM (visit takes 1 hour)

EVENING FREE

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Thursday Sept. 23rd

- 8:25 - 9:05 AM - Paul J. Gemperline
Modeling of Batch Processes With-In Spectroscopic and Calorimetric Measurements
- 9:05 - 9:30 AM - Ernesto Kriesten
Indirect Hard Modeling – A Method for the Analysis of Peak-shaped Signals of Reactive and Interacting Mixtures
- 9:30 - 9:55 AM - Roy Bruns
Unreplicated split-plot designs and approximate statistical models for the optimization of chemical systems
- 9:55 - 10:20 AM - Jacques Goupy
Which kind of Experimental Designs for finding and checking Robustness of Analytical Methods ?
- 10:20 - 11:00 AM - Coffee-break - POSTER SESSIONS 2,3 & 5
- 11:00 - 11:40 AM - Douglas N. Rutledge
Theory and Applications of the Principal Components Transform: A New Tool for Data Analysis
- 11:40 - 12:05 AM - António Barros
SegPCT-PLS: Segmented Principal Component Transform – Partial Least Squares regression.
- 12:05 - 12:30 AM - H.C.Smit
Optimum Separation, Information and Micro-miniaturisation. Considerations in the Signal Space.
- 12:30 AM - 1:30 PM - LUNCH – BUFFET served at HOLIDAY INN LISBON
- 1:30 - 2:10 PM - Bhavik R. Bakshi
Towards Bayesian Chemometrics - Promise and Problems
- 2:10 - 2:35 PM - Marco Reis
A comparative study of the performance of various linear regression methods in noisy environments
- 2:35 - 3:00 PM - Pierre Van Espen
Uncertainty assessment in bilinear and trilinear partial least squares.
- 3:00 - 3:25 PM - Federico Marini
On the use of a Kohonen neural network as a class-modeling tool.
- 3:25 - 3:40 PM - Coffee-break

**Thursday Sept. 23rd
(cont.)**

3:40 - 4:05 PM - Paul Geladi

Calibration standards: one-point, linear, nonlinear, multivariate, imaging, hyperspectral imaging and missing ones.

4:05 - 4:30 PM - M.H. Zhang

Boosting classification and regression trees

4:30 - 4:55 PM - Erik Skibsted

NAS SQC

4:55 - 5:35 PM - Anna de Juan

Protein processes: a challenging problem for multicomponent resolution and modelling.

5:35 - 5:50 PM

CAC-2006 Presentation

5:50 - 6:05 PM

CAC-2004 Closing Ceremony

AM	18 Saturday	19 Sunday	20 Monday	21 Tuesday	22 Wednesday	23 Thursday					
8:30			Opening	Plenary 5	Plenary 5	Plenary 3					
8:35			Plenary 1								
8:40				Oral 5	Oral 5	Oral 3					
8:45			Oral 1	Oral 5	Oral 5	Oral 3					
8:50			Oral 1	Oral 5	Oral 5	Oral 3					
8:55											
9:00	Pre-Conference Courses 1 & 4	Pre-Conference Courses 2, 3 & 6	POSTER	POSTER	POSTER	POSTER					
9:05											
9:10					SESSIONS	SESSIONS	SESSIONS				
9:15					1, 4 & 6	1, 4 & 6	2, 3 & 5				
9:20					Coffee Brk	Coffee Brk	Coffee Brk				
9:25					Plenary 1	Plenary 5	Plenary 4				
9:30					Oral 1	Oral 5	Oral 4				
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CEREMONY (opening, honoring, awarding, closing)

Poster Sessions with Coffee-Break

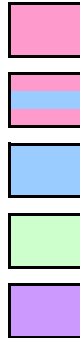
Coffee-Break / Leisure

Oral Presentation (25 min)

Oral Presentation (40 min)

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18 Saturday
Pre-Conference Courses 1, 4 & 5
Coffee Break
Pre-Conference Courses 1, 4 & 5



19 Sunday
Pre-Conference Courses 2, 3 & 6
Coffee Break
Pre-Conference Courses 2, 3 & 6

LISBON EXPERIENCE
Multimedia Show by the Tagus River
WELCOME PARTY by the TAGUS RIVER

20 Monday
Plenary 1
Oral 1
Oral 1
POSTER
SESSIONS
1, 4 & 6
Coffee Brk
Oral 5
Oral 5
Oral 5
Plenary 4
CHM History Session

21 Tuesday
Conference Tour (Lisbon, Cascais & Sintra)
Conference Banquet

22 Wednesday
Plenary 2
Oral 2
Oral 2
Oral 2
POSTER
SESSIONS
2, 3 & 5
Coffee Brk
Oral 2
Oral 2
Oral 2
Oral 2
Plenary 2
Poster Awards
LISBON OCEANARIUM

23 Thursday
Plenary 6
Oral 6
Oral 6
Oral 6
Oral 6
Coffee Break
Oral 6
Oral 6
Oral 6
Oral 6
Plenary 6
CAC-2006
CAC-2004 Closing Session