



# Хемометрика в аналитической ХИМИИ - 2008

Монпелье, Франция, 30 июня- 4 июля 2008 г.



**11<sup>th</sup> conference on Chemometrics  
in Analytical Chemistry (CAC-2008)**



# История проведения конференций

**Хемометрика** – химическая дисциплина, применяющая математические, статистические и другие методы, основанные на формальной логике, для построения или отбора методов измерения и планов эксперимента, а также для извлечения наиболее важной информации при анализе экспериментальных данных.

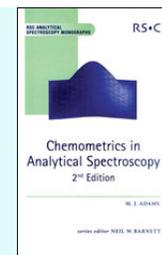
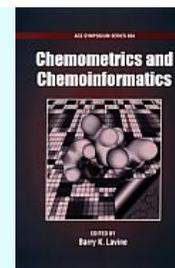
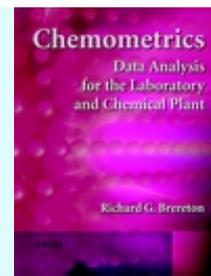
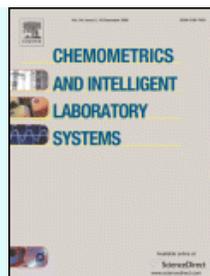
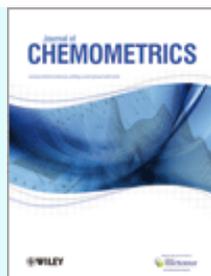
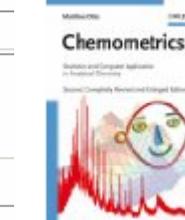
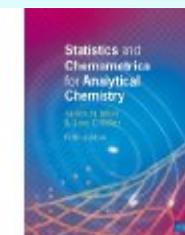
**D. Massart**

**Хемометрика** – синтетическая дисциплина, находящаяся на стыке химии и математики



# История проведения конференций

CAC	YEAR	DATE	COUNTRY	PLACE	COMMENTS
<a href="#">1 (I)</a>	1978	?	NETHERLANDS	Amsterdam	1st CAC
<a href="#">2 (II)</a>	1982	15-17 September	NETHERLANDS	Petten	
<a href="#">3 (III)</a>	1986	25-30 May	ITALY	Lerici	
<a href="#">4 (IV)</a>	1988	18-20 May	NETHERLANDS	Amsterdam	
<a href="#">5 (V)</a>	1992	14-17 July	CANADA	Montreal, Quebec	1st CAC not in Europe
<a href="#">6 (VI)</a>	1996	25-29 June	SPAIN	Tarragona, Catalonia	
<a href="#">7 (VII)</a>	2000	16-20 October	BELGIUM	Antwerp	
<a href="#">8 (VIII)</a>	2002	22-26 September	USA	Seattle, WA	
<a href="#">9 (IX)</a>	2004	20-23 September	PORTUGAL	Lisbon	Motto: New Challenges for a Maturing Science
<a href="#">10 (X)</a>	2006	10-15 September	BRAZIL	Águas de Lindóia, SP	1st CAC in the southern hemisphere. Motto: Chemometrics in the Tropics: Nature, Medicine and Industry
<a href="#">11 (XI)</a>	2008	30 June - 4 July	FRANCE	Montpellier	

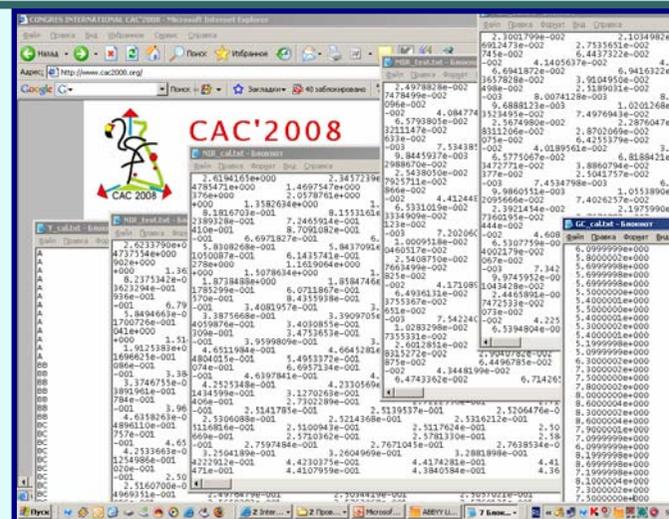




# Как получить возможность участвовать в конференции?

## 1. Chemometrics Shoot out

Обработка данных и построение модели для предсказания принадлежности образцов



## 2. Grants available to students

Документы:

- Подтверждение статуса студента
- Письмо от студента
- Тезисы для рецензирования

**Contribution Details**

Conference Track / Type of Submission: **Poster presentation**

**Chemometrics approach for simultaneous optimization of resolution, time of analysis and ruggedness of separation in MLC** **337**

**Boichenko, Alexander; Kulikov, A.U.; Galater.kharkov.ua, M.N.; Yakovleva, E.Yu.; Logunova, L.P.**  
Submitted by: Alexander Boichenko (kharkov.V.N. Karazin National University)

Presenting Author: Boichenko, Alexander (boichenko@univer.kharkov.ua)

Short CV of presenting author:  
A.P. Boichenko is a postgraduate student at Department of Chemical Metrology of Kharkov V.N. Karazin National University, Ukraine. His research interests include data analysis in analytical chemistry, metrology of quantitative analysis; retention modeling and optimization of separation in micellar and reversed-phase liquid chromatography.  
During last 3 years he has published 10 articles in such valuable journals such as Analytica Chimica Acta, J. Chromatogr. A, Chromatographia and have participated in International Conferences in Italy, Russia, Ukraine.

Topics: Advances in chemometrics  
Keywords: optimization of separation, retention modeling, Derringer's desirability function, ruggedness

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**Review Result of the Program Committee**

**The contribution has been accepted as poster**

Overview of Reviews

Questions	Review 1	Review 2
Familiarity of the reviewer with the topic	6	6
Recommendation	100%	8
Total points (out of 100)	80	100

# Сколько нужно денег для участия в международной конференции?

- **Регистрационный взнос:**

Normal price : 650 Euros + 50 Euros (Gala dinner) = 700 Euros

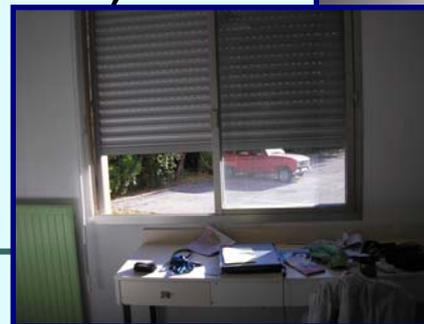
Early price : 450 Euros + 50 Euros (Gala dinner) = 500 Euros

Student price : 250 Euros + 50 Euros (Gala dinner) = 300 Euros

Accompanying person : 300 Euros + 50 Euros (Gala dinner) =  
350 Euros

e-conf : 100 Euros

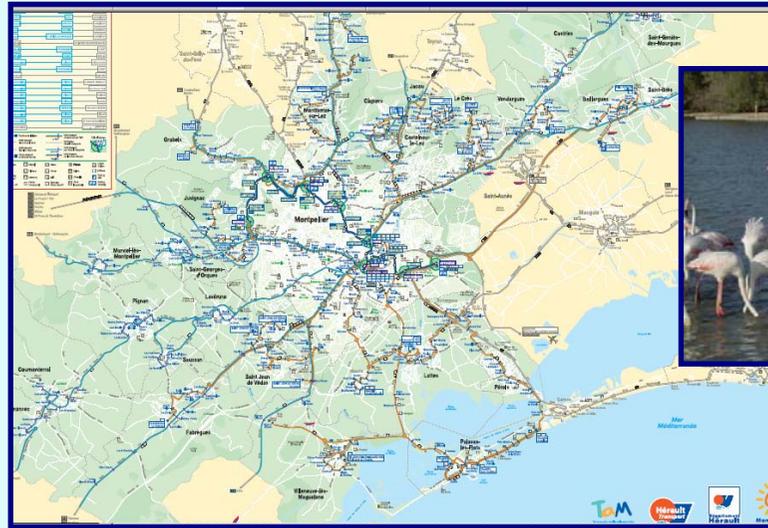
- **Проживание от 15 Евро/сутки  
(студенческое общежитие)**





# Montpellier

the city where the sun never sets





## Монпелье – место проведения конференции



**Монпелье - старинный французский город, расположенный в нескольких километрах от средиземного моря.**



# Монпелье – место проведения





# Тематика секций

- **Хемо- и биоинформатика**

Извлечение информации  
OMICS  
Планирование эксперимента  
Численное моделирование  
Прогресс в планировании эксперимента  
Изучение робастности  
Новые применения

- **Успехи в хемометрике**

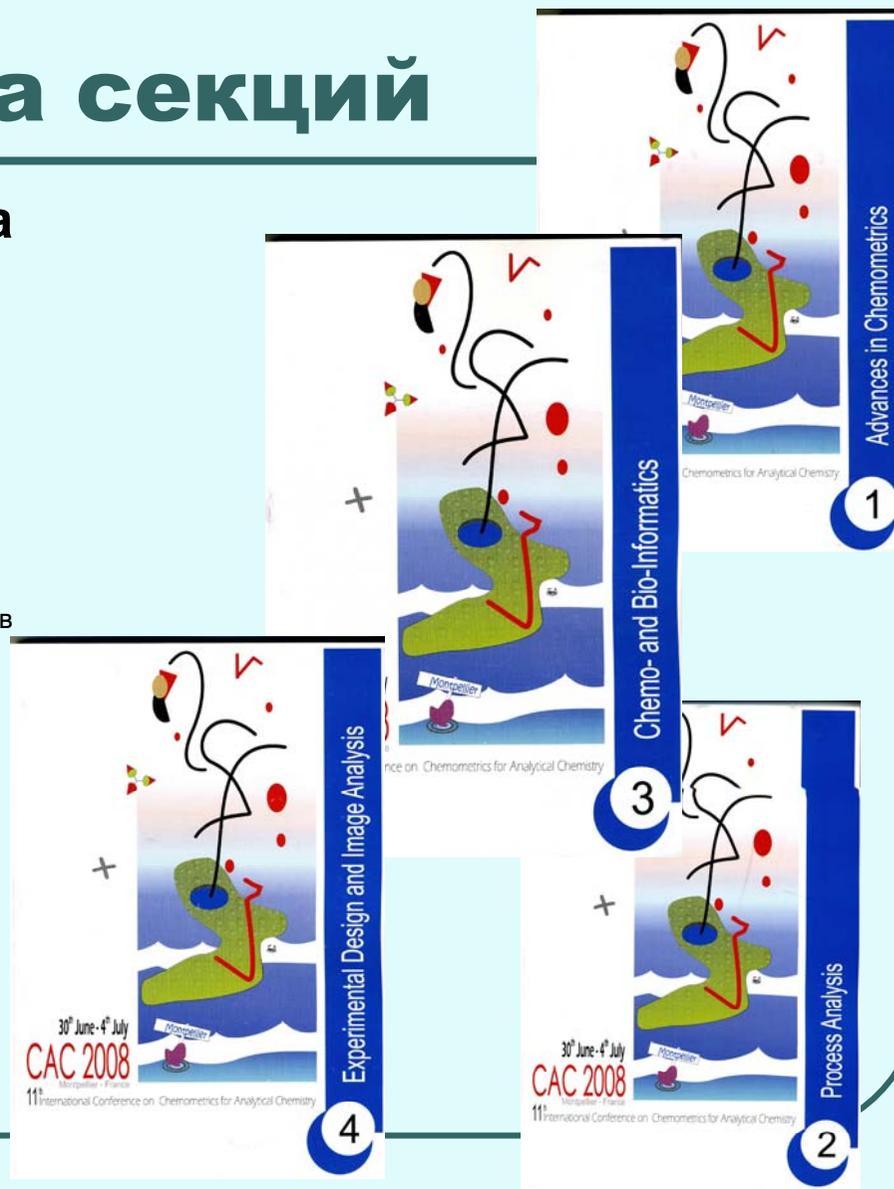
Разработка методов  
Улучшение точности, робастности, чувствительности, пределов обнаружения  
Новые применения

- **Анализ изображений**

Обработка изображений  
Сегментация  
Разрешение

- **Анализ процессов**

Моделирование и контроль процессов  
Диагностика в потоке  
Анализ в потоке





## Инновации в проведении и организации конференции

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- Возможность представления электронных постеров – небольших презентаций, которые периодически транслировались в залах
- 5 мин флэш-выступления молодых ученых без обсуждения в зале заседаний
- Электронная конференция
- Обсуждение интересных проблем между докладами
- Рецензирование всех докладов перед печатью в сборнике материалов
- Тезисы в виде коротких сообщений со структурой статей



## Пленарные доклады

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**Maria Celina Buydens**  
**Combining ANOVA and PCA in the analysis  
of microarray data**



**Ralf Marbach**  
**Adding value and safety to multivariate calibration  
by using SBC approach**



## Пленарные доклады

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**Magida Zeaiter**

**Process analytical technologies (PAT) tools for pharmaceutical process understanding and control – focusing on the science to achieve quality by design process.**



**John MacGregor**

**Process and product optimization using Latent variable models**



## Пленарные доклады

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**Johan Trygg**  
**Chemometrics in metabonomics and metabolomics**



**Jeremy Nicolson**  
**Statistical spectroscopy of metabolic supersystems**



## Пленарные доклады

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**Michelle Sergent**  
**Designs of experiments for robustness studies in analytical chemistry**



**Paul Geladi**  
**Multivariate and hyperspectral image analysis: overview and some special topics**



## Пленарные доклады

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**David Haaland**  
**Advanced approaches to multivariate curve  
resolution analysis of hyperspectral fluorescence  
images**



## Делегация из России



**Померанцев Алексей Леонидович**, Институт Химической  
Физики РАН  
Москва, Россия



**Родионова Оксана Евгеньевна**, Институт Химической  
Физики РАН  
Москва, Россия



**Кучерявский Сергей Владимирович**, Алтайский  
Государственный Университет  
Барнаул, Россия



**Богомоллов Андрей**, Гамбург, Германия



# Наш постер



## Chemometrics approach for simultaneous optimization of resolution, time of analysis, and ruggedness of separation in MLC

A.P. Boichenko,  
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**Micellar liquid chromatography (MLC)**

The equipment and columns for reversed-phase HPLC are used. Mobile phases are aqueous solutions of surfactants (very often sodium dodecyl sulfate (SDS)).

**ADVANTAGES OF MLC**

Nontoxic, nonflammable, enhanced fluorescent detection, simultaneous separation charged and uncharged analytes, separate separation of hydrophilic and hydrophobic analytes in one run, direct injection of physiological fluids.

**Problems**

Retention models for RP-HPLC are not valid for MLC. Theory of MLC is under construction. There are no approaches for simultaneous optimization of 3 main chromatographic goals: selectivity, time and ruggedness of separation.

## Interpretive chemometrics approach for optimization of selectivity, time of analysis, and ruggedness of separation in MLC

**Retention modelling in MLC**

**Three-phase distribution**

**Changing of solute microenvironment**

**New simple retention model**

On the basis of retention model that considering the changing of solute microenvironment on transferring from mobile to the stationary phase a new simple equation was proposed in MLC:

$$\log k' = a + b \log c_s + c \log c_m$$

The proposed retention model was tested and compared with other empirical and mechanistic models by using weighted least squares method to minimize the perturbation after Elution. Optimization and experimentally observed heteroscedasticity of retention factor in MLC.

The model gives the best values of adjusted and cross validated correlation coefficients.

**Selectivity of separation**

The separation factor was used as elementary resolution criterion for quantification of resolution between two neighboring peaks.

**Ruggedness**

The ruggedness was determined as mean of resolution variation in four directions.

**Time of analysis**

Time of analysis was determined as predicted retention time of last peak on the chromatogram.

**Combining of different chromatographic goals into single numerical value**

Normalization by Derringers desirability function

Calculation of Critical Response Function (CRF)

$$CRF_i = (R_{norm,i} \times T_{norm,i} \times RUG_{norm,i})^3$$

**Testing of the chemometrics approach**

**Separation of 14 food preservatives**

**Separation of flavanoids**

**Conclusions**

New optimization strategy for combining of three goals: resolution, time of separation and ruggedness was proposed in MLC. It based on: (i) collecting of experimental data in accordance with experimental design; (ii) modeling of retention of each component of mixture; (iii) estimation of quality of resolution; (iv) estimation of ruggedness of observed resolution; (v) taking into account the time of separation as one of optimization criteria; (vi) combining of the three values connected with resolution, time of separation, ruggedness of resolution into single numerical value by using Derringer's desirability function and plotting of surface plot of Critical Response Function; (vii) finding the optimal region of separation on the surface plot.

The proposed chemometrics approach was successfully applied for finding of optimal separation analysis conditions of 14 food preservatives and 13 flavanoids.



CAC'2008



# Французское меню (банкет)

## Clairette du Languedoc Adissan Rancio 1991

*Escalopes de foie gras poêlées aux raisins blancs et caramel de Carthage*

**Production location :** Adissan. This is the smallest and one of the oldest appellations of the Languedoc. It occupies the slopes bordering the middle valley of the Herault river.

**Grape variety :** Clairette 100%  
**Soil :** Villafranca terrace (ham soil)

**Vinification :** The grapes are separated just after manual harvesting. The grape skin maceration takes several days in order to obtain a strong colour. Maturation of 3 years minimum.

**Historical :** the wines of the Clairette have, one might say, always existed. First mentioned by Pliny the Ancien (in Gallo-Roman times) and later by Rabelais, it was particularly appreciated by Ronsard. It was classified PDO (Protected Designation of Origin) in 1948.

## Carte des vins

### Lucien Blanc 2006

*Filet de sebastie en portefeuille de tapenade verte et infusion de ciboulette*

**Production location :** Vint situated at an altitude of about 160m, at the foot of the Larzac hills.

**Grape variety :** Bourboulens, Marsanne, Grenache Blanc.

**Soils :** Clay stony with towards the slopes. Stri land parcels (DAO) (Native origin and qu

**Vinification:** maceration a controlled region of Lucian.

**Characteris** golden colour (fruity nose, on the palate perfumes Conserve in maximum. double this sea halve it.

### AOC la Clape 2005 "La Vendémiaire"

*Grenadin de veau à la crème de morilles*

**Production location :** Fleury d'Aude and Salles d'Aude. The Clape hills were at one time an island and are now a protected nature reserve. The

**Soils :** Clay stony with towards the slopes. Stri land parcels (DAO) (Native origin and qu

**Vinification:** maceration a controlled region of Lucian.

**Characteris** golden colour (fruity nose, on the palate perfumes Conserve in maximum. double this sea halve it.

## Menu

Des escalopes de foie gras poêlées aux raisins blancs et caramel de Carthage

...

Un filet de sebastie en portefeuille de tapenade verte et infusion de ciboulette

...

Un grenadin de veau à la crème de morilles

...

Un demi pelardon et confiture de figues

...

Un succés aux noisettes chocolat blanc

Kir à la fleur de mûre  
Vins AOC Languedoc  
Ronsardillon  
Calf

Conception et réalisation graphique : J.M.F. / C. G. / G. / G.





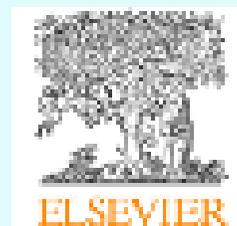
## Награждение лучших

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- The "best Shootout" award
  - The "best poster award"
  - The "best e-poster award"
  - The "best Junior Chemometrician award"
  - the "Best Chemometrician Award"
- Elsevier**



# Нужна ли хемометрика? – Спонсоры конференции





**Спасибо за внимание**

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