CHIMIA 50 (1996) Nr. 10 (Oktober)

# **Applications of Statistical Tools**

# Basler Sektion der Internationalen Biometrischen Gesellschaft (BBS)

# **Basle Section of the International Biometric Society (BBS)**

# Section Bâloise de la Société Internationale de Biométrie (SBB)

### **Date and Location**

Wednesday, 20.11.96, from 14.00 to 17.00 h Convention Center Basel

### Part 1: 14.00-15.30 h

### Statistical Experimental Design with Stavex

- Dr. Y.L. Grize, Ciba
  - 'Why and How to Study many Parameters Simultaneously?'
- · Dr. F. Petersen, Ciba
  - 'A Successful Stavex Application in Natural Substances Research'

#### Part 2: 15.30-17.00 h

## **QSAR** Analysis with Vesuv

· Dr. H. Schmidli, Ciba

'Optimization of Chemical Structures with Vesuv: Overview and Example'

Thanks to modern computer technology research chemists have today at their disposal user-friendly tools that allow them to exploit powerful statistical techniques such as statistical experimental design to optimally plan laboratory experiment or multivariate prediction to perform quantitative structure activity relationship analysis. These techniques will be briefly reviewed and two such tools: STAVEX and VESUV demonstrated on real examples.

**For further information** (final program, abstracts, facultative registration) please contact Dr. *Y.L. Grize*, Mathematical Applications in Chemistry and Physics, R-1008.Z2.05, *Ciba*, CH-4002 Basel.

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# 1st Swiss COST Chemistry Symposium

### Wednestay, 20th November 1996

## What is COST?

COST (a French acronym for 'Coopération Européenne dans le domaine de la recherche Scientifique et Technique') was set up in 1971 to stimulate and to give a framework for the European cooperation in the field of science and technology. This forum of research brings now together 25 European countries including the members of the European Union, of the EEE and seven central and eastern European states.

#### Why a 1st Swiss COST Chemistry Symposium?

The goal of this symposium is to present to the Swiss scientific public the progress of the research of the Swiss group in this European collaboration after three years of activities. The program consists of seven invited lectures by prominent European and Swiss scientists and 68 posters communications from Swiss scientists active in COST Chemistry.

### **Program**

All the abstracts have already been published in CHIMIA issue 7–8/96, p. 369–388.

## Welcome

- 10.00 Opening by Prof. André Merbach, Lausanne, Switzerland
- 10.05 Introduction by the Chairman of the Technical Committee Chemistry:

Prof. Gilbert Balavoine, CNRS, Toulouse, France

### **Lectures - Morning Session**

Chairman: Prof. Alexander von Zelewsky, Fribourg, Switzerland

- 10.15 Prof. Jan Reedijk, Leiden, The Netherlands 'Heavy Metal Compounds as Useful Drugs'
- 10.55 Prof. B. Giese, Basel, Switzerland 'Selectivity of Photochemical Cyclization Reactions with Amino Acids and Peptides'
- 11.35 Prof. Jürgen Brickmann, Darmstadt, Germany 'Modelling and Computer Simulation of Large Chemical Systems'

# Posters - Sandwich Session

12.15 Action D1: 'Coordination Chemistry in the Context of

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12.15 Action D1: 'Coordination Chemistry in the Context of

Biological and Environmental Studies'

Action D2: 'Selective Synthesis'
Action D3: 'Theory and Modelling of Chemistry Systems and Processes'

Action D4: 'Design and Preparation of New Molecular Systems with Unconventional Electrical, Optical and Magnetic Properties'

Action D5: 'Chemistry at Surfaces and Interfaces' Action D6: 'Chemical Processes and Reactions under

Extreme or Non Classic Conditions'

Action D7: 'Molecular Recognition Chemistry'

#### **Lectures – Afternoon Session**

Chairman: Prof. Hans-Ulrich Güdel, Berne, Switzerland Prof. Michael Grätzel, Lausanne, Switzerland 'Molecular Photovoltaics and Artificial Photosynthesis'

14.55 Prof. B. Delmon, Louvain-la-Neuve, Belgique 'From the Molecular Level to Chemical Engineering Models in Heterogeneous Catalysis. New Discoveries and Their Impact'

15.35 Coffee break

Prof. Richard R. Ernst, Zürich, Switzerland 16.00 'Nuclear Magnetic Resonance, a Powerful Tool for the Study of Biomolecular Dynamics'

16.40 Prof. Jean-Paul Behr, Illkirch, France 'The Proton Sponge: A Trick to Enter Cells the Viruses Didn't Exploit'

17.20 End of the Symposium

#### **Organization Committee**

T. Kaden (Basel), A. Merbach (Lausanne, Chairman), I. Portner (OFES, Bern), H.-P. Schelling (Sandoz, Basel), J. Weber (Geneva), J.-B. Weber (SNSF, Bern)

# For Correspondence

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