

EuCheMS-DAC Study Group / Task Force Annual Report for 2013-2014

Study Group / Task Force Name: Chemometrics
Study Group / Task Force Members and Affiliations: Romà Tauler, IDAEA-CSIC, Spain Federico Marini, University of La Sapienza, Rome, Italy Beata Walczak, University of Silesia, Katowice, Poland Lutgarde Buydens, Radboud University of Nijmegen, Netherlands Jean Michel Roger, IRSTEA CEMAGREF, Montpellier, France Alexey Pomerantsev/Oxana Radionova, Institute of Chemical Physics RAS, Moscow, Russia, Jan H Christensen, University of Copenhagen, Denmark Johan Trygg, University of Umeå, Sweden Richard Brereton, University of Bristol, England
Objectives: 1) Promote Chemometrics in Europe 2) Organize Chemometrics sessions in EuCheMS related conferences 2) Organize European Schools/Workshops on Chemometrics
Activities and Outputs in 2013-2014 (e.g. reports, publications, seminars, meetings): 1) Celebration of the chemometrics session during the celebration of Euroanalysis in 2013 (Monday 26 th August, 2013), at Warsaw. Beata Walczak from the University of Silesia took care of this organization, supported by the Polish Chemistry Society 2) Contribution to the European Analytical Column Nr 52 (attached) 'A personal view on chemometrics and analytical chemistry' by R.Tauler, F.Marini, B.Walczak, L.Buydens, R.G. Brereton, W. Buchberger and P.Worsfold, published in several analytical journals (ABC, TRAC,) 3) Finally it was not possible to organize a chemometrics session during the celebration of the EuCheMS congress in Istanbul, although attempted (it was not supported by the organizing committee)
Activities planned for 2014-2015: 1) Organization of a chemometrics session for analytical chemistry (if DAC agrees) during next Euroanalysis XVIII (6-10 Sept., 2015) in Bordeaux (France) 2) Preparation of EuCheMS session on chemometrics for omic sciences at next EuCheMS at Seville (2016) 3) Preparation of an European chemometrics school (planned but not achieved yet)
Report submitted by: Romà Tauler, (member of Catalan Chemistry Society and its former president)
Date submitted: 22 August 2014

DAC Chemometrics Study group

Chemometrics is the chemical discipline that uses mathematical and statistical methods to design or select optimal procedures and experiments, and to extract maximum chemical information by data-driven means. It is characterised by the application of mathematical, statistical and computer methods in order to address problems in chemistry, biochemistry, medicine, biology, environmental sciences and chemical engineering.

Chemometric techniques are heavily used in analytical chemistry and they are at present gaining increasing acceptance in emerging omic fields. The development of new chemometric methods continues to advance the state of the art in analytical instrumentation and methodology. It is an application driven discipline, and thus while the standard chemometric methodologies are very widely used in industry, academic groups are dedicated to the continued development of chemometric theory, method and application

- Objectives

- 1) Promote and Spread of Chemometrics in Europe
- 2) Organize Chemometrics sessions and workshops in EuChemS related conferences (and Euroanalysis)
- 2) Organize an European Schools/Workshops on Chemometrics

- Membership (new members will be asked to participate)

Romà Tauler, President of the Catalan Chemistry Society, IDAEA-CSIC, Spain

Federico Marini, University of La Sapienza, Rome, Italy

Beata Walczak, University of Silesia, Katowice, Poland

Lutgarde Buydens, Radboud University of Nijmegen, Netherlands

Jean Michel Roger, IRSTEA CEMAGREF, Montpellier, France / Douglas Rutledge, AgroParisTech, Paris, France

Alexey Pomerantsev/Oxana Radionova, Institute of Chemical Physics RAS, Moscow, Russia,

Jan H Christensen, University of Copenhagen, Denmark

Johan Trygg, University of Umeå, Sweden

Richard Brereton, University of Bristol, England

DAC Chemometrics study group

Aims and objectives

The aim of the Chemometrics study group is the promotion of Chemometrics in Europe through the organization of dedicated sessions in in EuCheMS related conferences and of European Schools/Workshops on Chemometrics

Chemometric techniques are heavily used in analytical chemistry and they are at present gaining increasing acceptance in emerging omic analytical fields. The development of new chemometric methods continues to advance the state of the art in analytical instrumentation and methodology. It is an application driven discipline, and thus while the standard chemometric methodologies are very widely used in industry, academic groups are dedicated to the continued development of chemometric theory, method and application.

Membership

Romà Tauler, President of the Catalan Chemistry Society, IDAEA-CSIC, Spain

Federico Marini, University of La Sapienza, Rome, Italy

Beata Walczak, University of Silesia, Katowice, Poland

Lutgarde Buydens, Radboud University of Nijmegen, Netherlands

Jean Michel Roger, IRSTEA CEMAGREF, Montpellier, France / Douglas Rutledge, AgroParisTech, Paris, France

Alexey Pomerantsev/Oxana Radionova, Institute of Chemical Physics RAS, Moscow, Russia,

Jan H Christensen, University of Copenhagen, Denmark

Johan Trygg, University of Umeå, Sweden

Richard Brereton, University of Bristol, England