

Study Group / Task Force Name: Chemometrics
Study Group / Task Force Members and Affiliations: Richard Brereton, University of Bristol, England Lutgarde Buydens / Jeroen Jansen (new incorporation), Radboud University of Nijmegen, Netherlands (Jan H Christensen, University of Copenhagen, Denmark Joao Lopes (new incorporation), Universidade de Lisboa, Lisbon, Portugal Federico Marini, University of La Sapienza, Rome, Italy Alexey Pomerantsev/Oxana Radionova, Institute of Chemical Physics RAS, Moscow, Russia, Jean Michel Roger, IRSTEA CEMAGREF, Montpellier, France; Douglas Rutledge, AgroParisTech / UMR1145 Ingénierie Procédés Aliments Romà Tauler, IDAEA-CSIC, Spain Johan Trygg, University of Umeå, Sweden Beata Walczak, University of Silesia, Katowice, Poland
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 2017-2018 (e.g. reports, publications, seminars, meetings): 1) Preparation of a session on chemometrics at EuCheMS session Liverpool, 29th August 2018, Room 4B Patter Recognition for Chemoemtrics and Metabolomics 14:00 - 14:30 AO25 Metabolomics for Clinical Analysis: Untargeted Diagnosis for an Unbiased Chemical Analysis Jeroen Jansen - Radboud University 14:30 - 15:00 AO26 Chemometrics for environmental omics Roma Tauler - IDAEA-CSIC 15:00 - 15:30 AO27 Multi-block approaches for a comprehensive metabolic characterization Federico Marini - University of Rome La Sapienza 16:00 - 16:30 AO28 Partial Least Square Discriminant Analysis : a much misunderstand and often misused technique for Metabolomics Richard Brereton - University of Bristol 16:30 - 17:00 AO29 Data Fusion in metabolomics Johan Trygg - Umea University 2) Writting 2nd part of the Feature Article for the ABC journal (see attached) Chemometrics in analytical chemistry—part II: modelling, validation and applications Richard G. Brereton, Jeroen Jansen, João Lopes, Federico Marini, Alexey Pomerantsev, Oxana Rodionova, Jean Michel Roger, Beata Walczak, Romà Tauler Analytical & Bioanalytical Chemistry, 2018, DOI: 10.1007/s00216-018-1283-4
Activities planned for 2018-2019: - Preparation of the chemometrics session and workshop/courses on chemometrics at Euroanalysis, September 2019, in Istanbul, Turkey - Continuing efforts to develop Chemometric schools at european level
Report submitted by: Romà Tauler
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