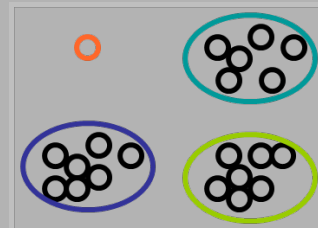
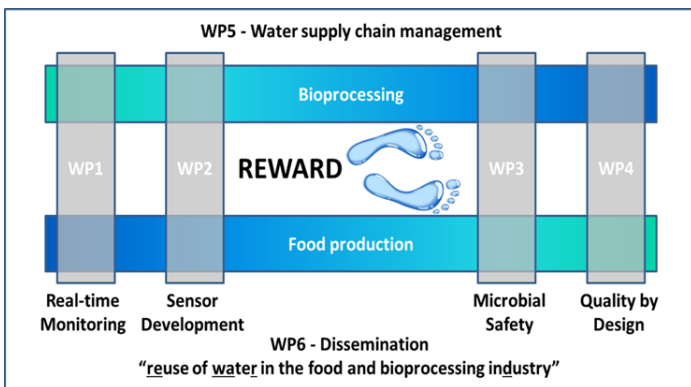


SPECTROSCOPY & CHEMOMETRICS



ISSUE 37 (OCTOBER-DECEMBER 2013)



REWARD - REUSE OF WATER IN THE FOOD AND BIOPROCESSING INDUSTRIES

SPECC (Søren B Engelsen & Frans van den Berg) in the lead of a 25 mio Dkr research project sponsored by the Strategic Research Council.

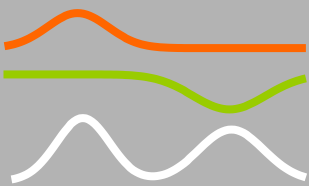
The project partners include DTU, TUM, ARLA and Novozymes and the main aim of REWARD is to reduce overall water consumption in the food and bioprocessing industries by reducing water intake and recycling of water streams. The primary tools adapted is the development and implementation of new sensors for in-line water monitoring, and the application of Process Analytical Technology and Quality by Design methodologies.

BIOPRO - WORLD TALENT CAMPUS

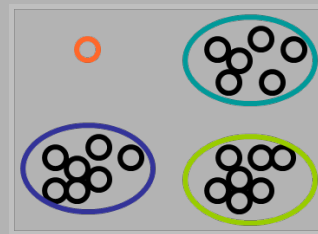
SPECC (Frans van den Berg) major contributor to the BIOPRO world talent campus at the Mærsk Mc-Kinney Møller Science Center in Sorø. The participants have all gone through an application process before being selected for WTC course by the BIOPRO steering committee. The students have been awarded 3 ECTS-points.

Picture: The winning team with their LEGO prize: Hilde Larsson, Technical University of Denmark, Stephen Goldrick, Newcastle University, Aditya Kunjapur, Massachusetts Institute of Technology, Laura Jeffrey, University of Strathclyde and Tobias Ladner, Aachen University.

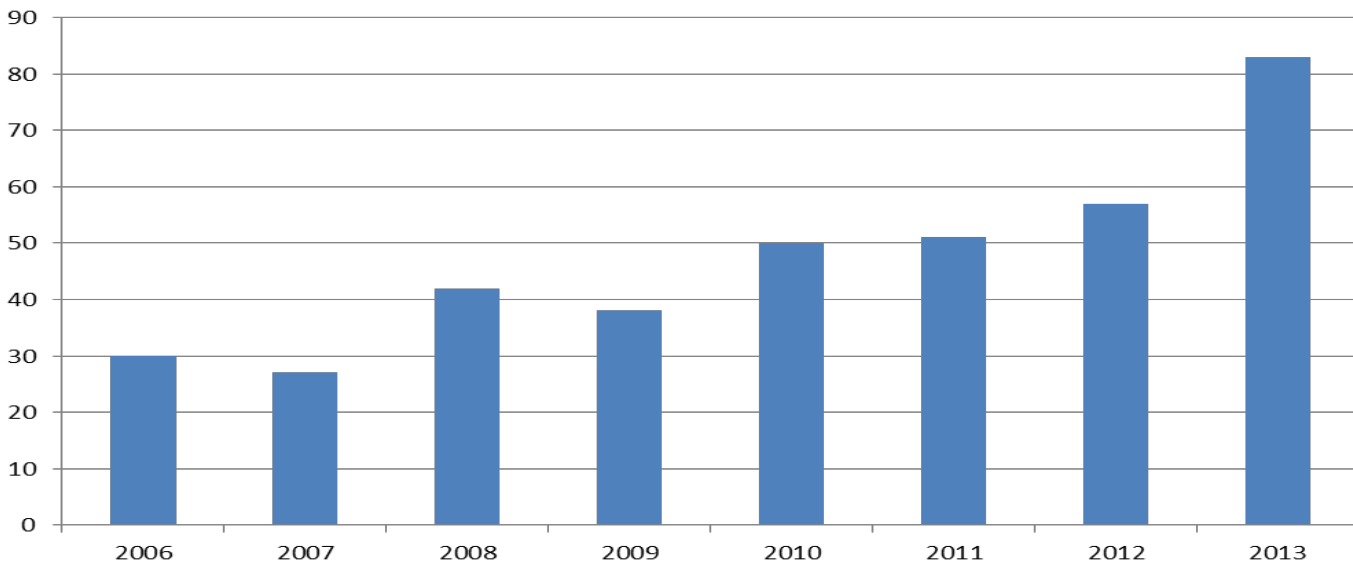




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SPECC peer reviewed publications



Peer reviewed publications Oct-Dec 2013:

KR Murphy, CA Stedmon, D Graeber, R Bro. Fluorescence spectroscopy and multi-way techniques. *PARAFAC. Analytical Methods*. 5 (23), 6541–6882, 2013.

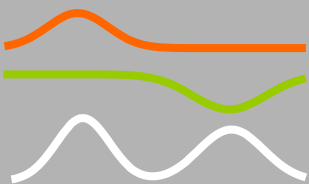
E Acar, MA Rasmussen, F Savorani, T Næs, R Bro. Understanding data fusion within the framework of coupled matrix and tensor factorizations. *Chemometrics and Intelligent Laboratory Systems*. 129, 53–63, 2013.

R Di Salvo, C Fadda, AM Sanguinetti, T Næs, A Del Caro. Effect of harvest time and geographical area on sensory and instrumental texture profile of a PDO artichoke. *International Journal of Food Science and Technology*. 49 (1), 1-7, 2013.

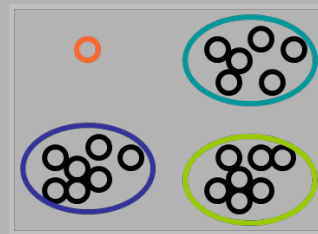
EE Papalexakis, ND Sidiropoulos, R Bro. From *K*-Means to Higher-Way Co-Clustering: Multilinear Decomposition With Sparse Latent Factors. *IEEE Transactions on signal processing*. 61 (2), 493-506, 2013.

M van Maarschalkerweerd, R Bro, M Egebo, S Husted. Diagnosing Latent Copper Deficiency in Intact Barley Leaves (*Hordeum vulgare*, L.) Using Near Infrared Spectroscopy. *Journal of Agricultural and Food Chemistry*. 61 (46), 10901–10910, 2013.

MS Andersen, HC Reinbach, Å Rinnan, T Barri, C Mithril, LO Dragsted. Discovery of exposure markers in urine for Brassica-containing meals served with different protein sources by UPLC-qTOF-MS untargeted metabolomics. *Metabolomics*. 9 (5), 984–997, 2013.



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Peer reviewed publications Oct-Dec 2013:

JV Räsänen, T Holopainen, J Joutsensaari, C Ndamb, P Pasanen, Å Rinnan, M Kivimäenpää. Effects of species-specific leaf characteristics and reduced water availability on fine particle capture efficiency of trees. *Environmental Pollution*. 183, 64-70, 2013.

S Hoff, MN Lund, MA Petersen, W Frank, ML Andersen. Storage stability of pasteurized non-filtered beer. *Journal of the Institute of Brewing*. 119 (3) 172–181, 2013.

B Khakimov, MS Motawia, S Bak, SB Engelsen. The use of trimethylsilyl cyanide derivatization for robust and broad-spectrum high-throughput gas chromatography–mass spectrometry based metabolomics. *Analytical and Bioanalytical Chemistry*. 405 (28), 2013.

LB Lyndgaard, F van den Berg, A de Juan. Quantification of paracetamol through tablet blister packages by Raman spectroscopy and multivariate curve resolution-alternating least squares. *Chemometrics and Intelligent Laboratory Systems*. 125, 58–66, 2013.

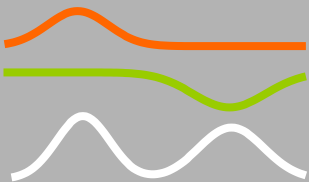
SB Petersen, MA Rasmussen, M Strøm, TI Halldorsson, SF Olsen. Sociodemographic characteristics and food habits of organic consumers – a study from the Danish National Birth Cohort. *Public Health Nutrition*. 16 (10), 1810–1819, 2013.

C Piras, FC Marincola, F Savorani, SB Engelsen, S Cosentino, S Viale, MB Pisano. A NMR metabolomics study of the ripening process of the Fiore Sardo cheese produced with autochthonous adjunct cultures. *Food Chemistry*. 141 (3), 2137–2147, 2013.

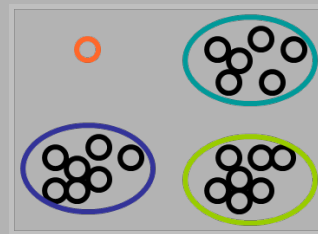
F Marini, R Bro. SCREAM: A novel method for multi-way regression problems with shifts and shape changes in one mode. *Chemometrics and Intelligent Laboratory Systems*. 129, 64–75, 2013.

FJ McEvoy, C Henriksson, C Obel, DH Nielsen, JM Amigo. Automated Localization of the Femoral Head Center on Pelvis Radiographs. *Veterinary Radiology and Ultrasound*. 56 (6), 680-698, 2013.

L Paudel, RW Adams, P Király, JA Aguilar, M Foroozandeh, MJ Cliff, M Nilsson, P Sándor, JP Waltho, GA Morris. Simultaneously Enhancing Spectral Resolution and Sensitivity in Heteronuclear Correlation NMR Spectroscopy. *Angewandte Chemie International Edition*. 52 (44), 11616 –11619, 2013.



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Peer reviewed publications Oct-Dec 2013:

AA Colbourne, S Meier, GA Morriss, M Nilsson. Unmixing the NMR spectra of similar species – vive la difference. *Chemical Communications*. 49 (89), 10510-10512, 2013.

F Savorani, MA Rasmussen, MS Mikkelsen, SB Engelsen. A primer to nutritional metabolomics by NMR spectroscopy and chemometrics. *Food Research International*. 54 (1), 1131–1145, 2013.

S Ibrügger, M Kristensen, MW Poulsen, MS Mikkelsen, J Ejsing, BM Jespersen, LO Dragsted, SB Engelsen, S Bügel. Extracted Oat and Barley β -Glucans Do Not Affect Cholesterol Metabolism in Young Healthy Adults. *The Journal of Nutrition*. 143, 1579-1585, 2013.

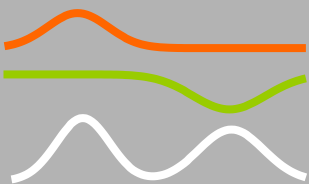
E Menichelli, M Hersleth, T Almøy, T Næs. Alternative methods for combining information about products, consumers and consumers' acceptance based on path modelling. *Food Quality and Preference*. 31, 142–155, 2013.

L Louw, S Malherbe, T Næs, M Lambrechts, P van Rensburg, H Nieuwoudt. Validation of two Napping techniques as rapid sensory screening tools for high alcohol products. *Food Quality and Preference*. 30 (2), 192–201, 2013.

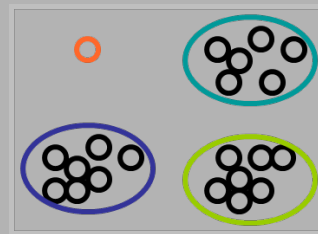
JM Amigo. Emerging possibilities of near infrared spectroscopy and near infrared chemical imaging in the pharmaceutical manufacturing industry. The challenge of the process analytical technologies paradigm or just a research tool. *NIRnews*. 24 (8), 9-12, 2013.

Other publications Oct-Dec 2013:

DT Berhe, MS Hviid, SB Engelsen, R Lametsch. Use of Raman spectroscopy to study effect of cooking temperature and time on meat proteins. *59th International Congress of Meat Science and Technology*. 1-4, 2013.



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Other publications Oct-Dec 2013:

Å Rinnan, JM Amigo, T Skov. Multiway methods in food science. In: *Mathematical and Statistical Methods in Food Science and Technology*. Chapter 9. 143-174, 2013.

M Egebo, Å Rinnan, SB Engelsen, R Bro, L Nørgaard. New chemometric methods for solving classification problems in NIR spectroscopy. In: *Proceedings of the 15th International Conference on Near Infrared Spectroscopy*. 1-4, 2013.

Å Rinnan, MO Andersson, C Ridder, SB Engelsen. Recursive weighted PLS (rPLS): an efficient and promising multivariate method for spectral variable selection in regression. In: *Proceedings of the 15th International Conference on Near Infrared Spectroscopy*. 1-5, 2013.

E Acar, AJ Lawaetz, MA Rasmussen, R Bro. Structure-Revealing Data Fusion Model with Applications in Metabolomics. Conference: *35th Annual International Conference of the IEEE EMBS Osaka, Japan*. 6023-6026, 2013.

E Salvatore, M Bevilacqua, R Bro, F Marini, M Cocchi. Classification Methods of Multiway Arrays as a Basic Tool for Food PDO Authentication. In: *Comprehensive Analytical Chemistry*. 60, 339-382, 2013.

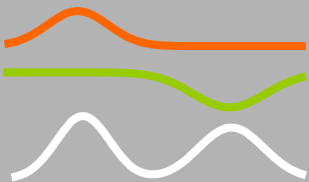
L Nørgaard, SB Engelsen, R Bro. Vi har siden december 2007 haft fornøjelsen af at skrive en månedlig klumme i Dansk Kemi. Tiden er moden til at afslutte disse, og vi vil gerne sige tak for denne gang. *Dansk Kemi. Det Kemometriske Rum*. 94 (8), 30-31, 2013.

SB Engelsen. Søren Balling Engelsen. Interview in: *NIRnews*. 24 (7), 10-14, 2013.

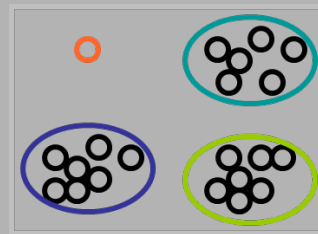
A del Olmo, JM Amigo, M Møller, SB Engelsen. Spatial distribution of staling of white wheat bread as studied by texture analyzer, classical NIR and hyperspectral imaging. *NIR2013*. 2013.

S Grassi, JM Amigo, C Lyndgaard, I Vigentini, E Casiraghi. Beer fermentation monitoring by using FT-NIR spectroscopy. *NIR2013*. 2013.

S Grassi, C Alamprese, V Bono, C Picozzi, R Foschino, E Casiraghi, JM Amigo. MCR applied to milk lactic acid fermentation monitoring. *NIR2013*. 2013.



SPECTROSCOPY & CHEMOMETRICS



Staff:

- Tine Ringsted, PhD student 1/10 2013 – 30/9 2016 (SB Engelsen)
- Ningchuan Wang, MSc student 11/11 2013 – 10/8 2014 (F van den Berg)
- Marie Wolsing, MSc student 1/12 2013 – 30/5 2014 (F van den Berg)
- Katharina Böckmann, MSc student 1/12 2013 – 30/5 2014 (F van den Berg)
- Anders Juul Lawaetz, post doc 1/12 2013 – 30/11 2014 (Å Rinnan)

Guest Researchers:

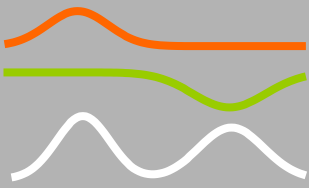
- Claudia Di Ciero (host F Savorani, 6/11 2013 – 28/2 2014)
- Bashar Amer (host T Skov, 2/12 2013 – 31/1 2014)

PhD defences:

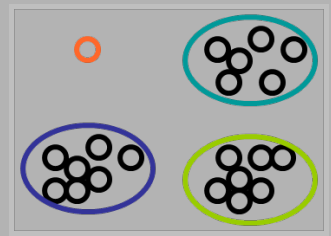
- **Bekzod Khakimov** (supervisor SB Engelsen): Metabolomics and bioactive substances in plants. November 8th, 2013
- **Signe Hoff** (supervisor BM Jespersen): From Barley to Beer Oxidation throughout the brewing process. November 22nd, 2013
- **Maja Kamstrup-Nielsen** (supervisor R Bro): Metabolomics from a chemometric point of view. November 25th, 2013
- **Lotte Bøge Lyndgaard** (supervisor F van den Berg): Applications of Raman Spectroscopy and Multivariate Data Analysis in Food and Pharmaceutical Sciences. December 16th, 2013

BSc & MSc defences:

- Marietta Kokla (supervisor JM Amigo): Detection of pulmonary thrombosis in dogs using texture analysis and multivariate classification models. December 13th, 2013



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Courses: (Oct-Dec)

Block 2:

- Advanced Chemometrics (MA Rasmussen, T Skov, R Bro, 20 students)
- Quantitative Bio-spectroscopy (N Viereck, SB Engelsen, FH Larsen, 19 students)
- Plant Polysaccharides: Biology, Structure and Applications (FH Larsen, SB Engelsen, 8 students)
- Brewing 1 (BM Jespersen, F van den Berg, 16 students)
- PhD: Quantitative Food Spectroscopy (N Viereck, SB Engelsen, FH Larsen, 1 student)
- ODIN: NIR Spectroscopy 10/10
- ODIN: Basic Chemometrics 21-22/10
- ODIN: Multiway Analysis 29-30/10
- ODIN: A day of 100 Methods 9/12

New granted projects:

- **REWARD** – REuse of WAtER in the food and bioprocessing inDUstry. Søren Balling Engelsen and Frans van den Berg, The Danish council for strategic research
- **RenPåNy**. Frans van den Berg and Nanna Viereck, Grønt Udviklings- og Demonstrationsprogram (GUDP)