SPECTROSCOPY & CHEMOMETRICS

ISSUE 36 (JULY-SEPTEMBER 2013)

NEW NAME OF SECTION: At the recently held GRUS it was decided to change our name to SPECtroscopy & Chemometrics:

SPECC

IN A PITCH CONTEST in which 12 PhD students and researchers were given five to seven minutes to present their research project and its value for the food industry, SPECC PhD student Carl Emil Eskildsen won for his pitch with focus on development of a rapid method for prediction of quality parameters in milk. The pitches were evaluated by a panel of four persons from the industry and trade organisations. At the picture, Carl Emil receives the award by Thomas Mathiasen, CEO TM-Innovation.

Spectroscopy & Chemometrics
Department of Food Science
Faculty of Science
University of Copenhagen

Rolighedsvej 30
DK - 1958 Frederiksberg C
Phone + 45 35 33 32 39
www.models.life.ku.dk

Peer reviewed publications July-Sept 2013:

G Azevedo, L Hilliou, G Bernardo, I Sousa-Pinto, RW Adams, M Nilsson, RD Villanueva. Tailoring kappa/iota-hybrid carrageenan from *Mastocarpus stellatus* with desired gel quality through pre-extraction alkali treatment. *Food Hydrocolloids*. 31 (1), 94-102, 2013.

BR Martini, VA Mandelshtam, GA Morris, AA Colbourne, M Nilsson. Filter diagonalization method for processing PFG NMR data. *Journal of Magnetic Resonance*. 234, 125-134, 2013.

B Ibrahim, P Marsden, JA Smith, A Custovic, M Nilsson, SJ Fowler. Breath metabolomic profiling by nuclear magnetic resonance spectroscopy in asthma. *Allergy*. 68 (8), 1050-1056, 2013.

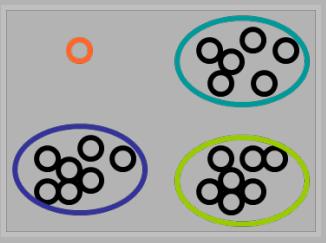
R Evans, Z Deng, AK Rogerson, AS McLachlan, JJ Richards, M Nilsson, GA Morris. Quantitative Interpretation of Diffusion-Ordered NMR Spectra: Can We Rationalize Small Molecule Diffusion Coefficients? *Angewandte Chemie-international Edition* 52 (11), 3199-3202, 2013.

DJ Codling, G Zheng, T Stait-Gardner, S Yang, M Nilsson, WS Price. Diffusion Studies of Dihydroxybenzene Isomers in Water−Alcohol Systems. *The Journal of Physical Chemistry*. 117 (9), 2734-2741, 2013.

S Islam, JA Aguilar, MW Powner, M Nilsson, GA Morris, JD Sutherland. Detection of Potential TNA and RNA Nucleoside Precursors in a Prebiotic Mixture by Pure Shift Diffusion-Ordered NMR Spectroscopy. *Chemistry*. 19 (14), 4586-4595, 2013.

RW Adams, CM Holroyd, JA Aguilar, M Nilsson, GA Morris. ‘‘Perfecting’’ WATERGATE: clean proton NMR spectra from aqueous solution. *Chemical Communications* 49, 358-360, 2013.

G Gürdeniz, L Hansen, MA Rasmussen, E Acar, A Olsen, J Christensen, T Barri, A Tjønneland, LO Dragsted. Patterns of time since last meal revealed by sparse PCA in an observational LC–MS based metabolomics study. *Metabolomics*. 9 (40), 1-9, 2013.



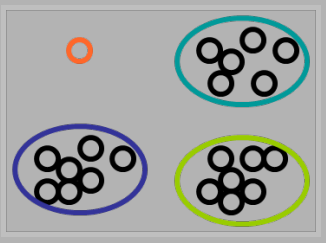
Peer reviewed publications July-Sept 2013:

M Owusu, MA Petersen, H Heimdal. Relationship of sensory and instrumental aroma measurements of dark chocolate as influenced by fermentation method, roasting and conching conditions. *Journal of Food Science and Technology*. 50(5), 909–917, 2013.

C Varming, MA Petersen, TB Toldam-Andersen. Ascorbic acid contents in Danish apple cultivars and commercial apple juices. *LWT - Food Science and Technology*. 54 (2), 597-599, 2013.

H Babamoradi, F van den Berg, Å Rinnan. Comparison of bootstrap and asymptotic confidence limits for control charts in batch MSPC strategies. *Chemometrics and Intelligent Laboratory Systems*. 127, 102-111, 2013.

AD Bond, C Cornett, FH Larsen, H Qu, D Raijada, J Rantanen. Interpreting the Disordered Crystal Structure of Sodium Naproxen Tetrahydrate. *Crystal Growth & Design*. 13 (8), 3665-3671, 2013.



Other publications:

M Egebo, . 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*. 87-90, 2012.

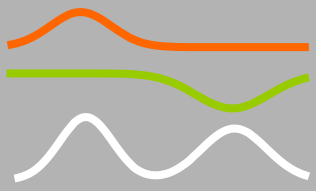
Å Rinnan, MO Andersson, C Ridder, SB Engelsen. Recursive weighted PLS (rPLS): an efficient and promising multivariate method for spectral variable selection in regression, In: *Proceedings of the 15th International Conference on Near Infrared Spectroscopy*. 91-95, 2012.

E Acar, G Lozanski, MN Gurcan. Tensor-based Computation and Modeling in Multi-resolution Digital Pathology Imaging: Application to Follicular Lymphoma Grading. *Conference: Medical Imaging 2013*. 8676, 2013.

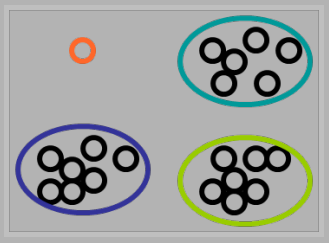
F Savorani, MA Rasmussen, Å Rinnan, SB Engelsen. Interval-Based Chemometric Methods in NMR Foodomics. In: *Chemometrics in Food Chemistry 28.* 449-486, 2013.

Media:

-



SPECTROSCOPY & CHEMOMETRICS



Staff:

- Maria Francisca Folque Gouveia, PhD student 1/9 2013 – 31/8 2016 (R Bro)
- Alessandra Biancolillo, PhD student 1/9 2013 – 31/8 2016 (R Bro)
- Bekzod Khakimov, post doc 1/9 2013 – 31/8 2014 (SB Engelsen)
- Lotte Bøge Lyndgaard, post doc 20/9 2013 – 20/3 2014 (T Skov)
- Mette Holse, post doc 1/9 2013 – 31/8 2016 (BM Jespersen)

Guest Researchers:

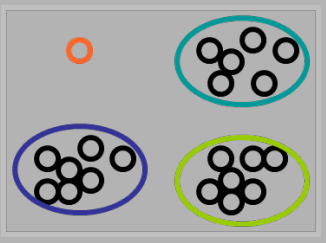
- Marta Bevilacqua (host R Bro, 15/8 – 1/10 2013)
- Ane Bordagaray (host JM Amigo, 1/9 – 1/12 2013)
- Maria Angeles, (host JM Amigo, 1/9 – 1/10 2013)
- Alexandra Andrei (host R Bro, 2/9 2013 – 1/4 2014)

PhD defences:

- Anja Niehues Birch (supervisor ÅS Hansen): Aroma of wheat bread crumb - effect of fermentation temperature and baker's yeast. July 1st, 2013.

BSc & MSc defences:

- Carl Emil Aae Eskildsen (supervisor T Skov): Quantification of fatty acid profile in milk - challenges using FT-IR and chemometrics. September 20th, 2013.



Courses:

- Basic Course in Food Science (MA Petersen, SB Engelsen, BM Jespersen, 120 students, block 1)
- Exploratory Data Analysis (Å Rinnan, 53 students, block 1)
- Design of Experiments and Optimization (F van den Berg, 30 students, block 1)
- Fundamentals of Beer Brewing and Winemaking (FH Larsen, MA Petersen, 25 students, block 1)
- PhD: Introduction to MATLAB for Multivariate Data Analysis (JM Amigo, 21 students, block 1)
- PhD: Multi-way analysis (R Bro, 10 students, block 1)
- PhD: Hyperspectral and Multichannel Image Analysis (JM Amigo, 15 students, block 1)
- PhD: Copenhagen School of Chemometrics – CSC (JM Amigo, 35 students, block 1)
- ODIN: Design of experiments 16-17/9
- ODIN: Fluorescence spectroscopy 20/9

New granted projects:

-