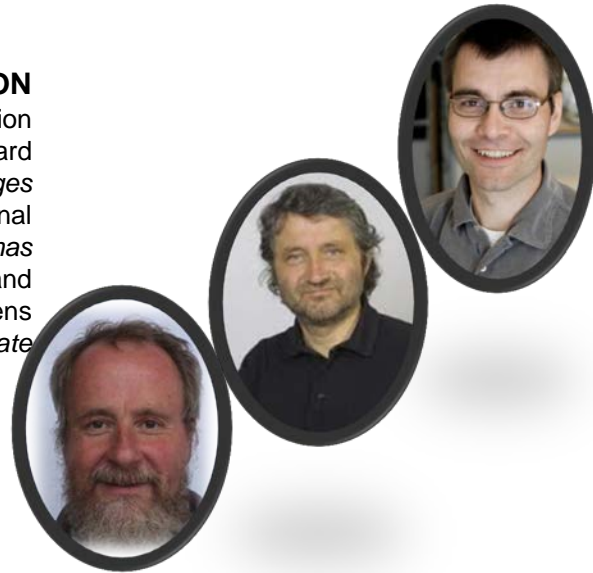


ISSUE 31 (APRIL-JUNE 2012)

THE COPENHAGEN CHEMOMETRIC SESSION

April 26th Q&T hosted the 1st Copenhagen Chemometric Session beginning with the Inargural lecture by Professor Lars Nørgaard "Chemometrics - exploration and solution of complex challenges in research and development", followed up by a confessional lecture by Professor Tormod Næs entitled "What has chemometrics taught me? Confessions from a statistician" and finishing with a Honorary lecture by professor Harald Martens entitled "Chemometrics in applied mathematics: multivariate metamodelling"

We greatly indebted to the speakers who made the event memorable and the event worth continuing.



Peer reviewed publications:

LG Rasmussen, H Winning, F Savorani, C Ritz, SB Engelsen, A Astrup, TM Larsen, LO Dragsted. Assessment of dietary exposure related to dietary GI and fibre intake in a nutritional metabolomic study of human urine. *Genes & Nutrition*. 7 (2), 281-293, 2012.

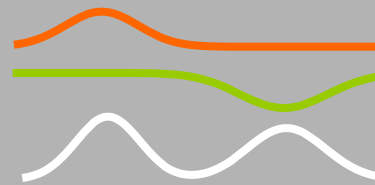
CA Daykin, R Bro, F Wulfert. Data handling for interactive metabolomics: tools for studying the dynamics of metabolome-macromolecule interactions. *Metabolomics*. 8 (4), 52-63, 2012.

A Digaitiene, ÅS Hansen, G Juodeikiene, D Eidukonyte, J Josephsen. Lactic acid bacteria isolated from rye sourdoughs produce bacteriocin-like inhibitory substances active against *bacillus subtilis* and fungi. *Journal of Applied Microbiology*. 112 (4), 732-742, 2012.

LB Lyndgaard, K Sørensen, FWJ van der Berg, SB Engelsen. Depth profiling of porcine adipose tissue by Raman spectroscopy. *Journal of Raman Spectroscopy*. 43 (4), 482-489, 2012.

AJ Lawaetz, R Bro, MH Kamstrup-Nielsen, IJ Christensen, LN Jørgensen, HJ Nielsen. Fluorescence spectroscopy as a potential metabonomic tool for early detection of colorectal cancer. *Metabolomics*. 8 (1), 111-121, 2012.

L Nuobariene, ÅS Hansen, N Arneborg. Isolation and identification of phytase-active yeasts from sourdoughs. *LWT - Food Science and Technology*. 48 (2), 190-196, 2012.



Peer reviewed publications:

FH Larsen, M Schöbitz, J Schaller. Hydration properties of regioselectively etherified celluloses monitored by ^2H and ^{13}C solid-state MAS NMR spectroscopy. *Carbohydrate Polymers*. 89 (2), 640–647, 2012.

M Hølse, T Skov, ÅS Hansen. Oxidative storage stability of roasted maramba beans (*Tylosema esculentum*). *Food Research International*. 47 (2), 385–391, 2012.

A Gredilla, JM Amigo, SF de Vallejuelo, A de Diego, R Bro, J Madariaga. Practical comparison of multivariate chemometric techniques for pattern recognition used in environmental monitoring. *Analytical Methods*. 4 (3), 676-684, 2012.

N Ratola, JM Amigo, S Lacorte, D Barceló, E Psillakis, A Alves. Comparison of PAH levels and sources in pine needles from Portugal, Spain, and Greece. *Analytical Letters*. 45 (5-6), 508-525, 2012.

S Hoff, ML Lametsch, MA Petersen, BPM Jespersen, ML Andersen. Influence of malt roasting on the oxidative stability of sweet wort. *Journal of Agricultural and Food Chemistry*. 60 (22), 5652-5659, 2012.

E López-Rituerto, F Savorani, A Avenozza, JH Busto, JM Peregrina, SB Engelsen. Investigations of La Rioja terroir for wine production using ^1H NMR metabolomics. *Journal of Agricultural and Food Chemistry*. 60 (13), 3452-3461, 2012.

JX Wu, D Xia, FWJ van den Berg, JM Amigo, T Radesa, M Yanga, J Rantanen. A novel image analysis methodology for online monitoring of nucleation and crystal growth during solid state phase transformations. *International Journal of Pharmaceutics*. 433 (1-2), 60–70, 2012.

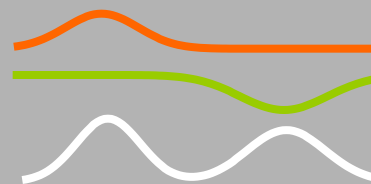
C Garrido-Novell, D Pérez-Marin, JM Amigo, J Fernández-Novales, JE Guerrero, A Garrido-Varo. Grading and color evolution of apples using RGB and hyperspectral imaging vision cameras. *Journal of Food Engineering*. 113 (2), 281–288, 2012.

M Brydegaard, A Runemark, R Bro. Chemometric approach to chromatic spatial variance. Case study: patchiness of the Skyros wall lizard. *Journal of Chemometrics*. 26 (6), 246-255, 2012.

M Kristensen, MG Jensen, MS Mikkelsen, A Astrup. Flaxseed dietary fibers lower cholesterol and increase fecal fat excretion, but magnitude of effect depend on food type. *Nutrition & Metabolism*. 9 (8), 2012.

S Ibrügger, M Kristensen, MS Mikkelsen, A Astrup. Flaxseed dietary fiber supplements for suppression of appetite and food intake. *Appetite*. 58 (2), 490-495, 2012.

N Ratola, JM Amigo, S Lacorte, D Barceló, E Psillakis, A Alves. “Biomonitoring of Polycyclic Aromatic Hydrocarbons by Pine Needles – Levels and Trends in Southern Europe” In: *Polycyclic Aromatic Hydrocarbons: Chemistry, Occurrence and Health Issues*. 978-1-62257-473-5, 2012.



Other publications:

R Bro, SB Engelsen, L Nørgaard. Multivejs-vekselvirkninger: Tusker3-modellering. *Dansk Kemi. Det Kemometriske Rum.* 93, (6/7), 24-25, 2012.

R Bro, SB Engelsen, L Nørgaard. Når PARAFAC ikke virker. *Dansk Kemi. Det Kemometriske Rum.* 93, (5), 43-44, 2012.

SB Engelsen, R Bro, L Nørgaard. PARAFAC, NMR og lipoproteiner. *Dansk Kemi. Det Kemometriske Rum.* 93 (4), 32-33, 2012.

R Bro, B Pedersen. Kemometriens mange muligheder. *Aktuel Naturvidenskab.* 2, 28-31, 2012.

A Gowen, JM Amigo. Applications of Spectroscopy and Chemical Imaging in Pharmaceuticals. In: *Handbook of Biophotonics.* 3 (1), 71-86, 2012.

MS Mikkelsen. Large-scale extraction and molecular analysis of cereal β -glucan. *International Association for Cereal Science and Technology (ICC)* 2012.

External publications:

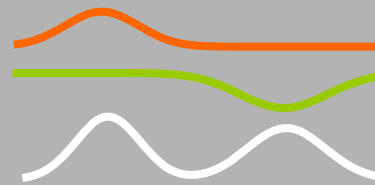
CF Tormena, R Evans, S Haiber, M Nilsson, GA Morris. Matrix-assisted diffusion-ordered spectroscopy: application of surfactant solutions to the resolution of isomer spectra. *Magnetic Resonance in Chemistry.* 50, (6), 458-465, 2012.

J Cassani, M Nilsson, GA Morris. Flavonoid Mixture Analysis by Matrix-Assisted Diffusion-Ordered Spectroscopy. *Journal of Natural Products.* 75, 131-134, 2012.

JA Aguilar, AA Colbourne, J Cassani, M Nilsson, GA Morris. Decoupling Two-Dimensional NMR Spectroscopy in Both Dimensions: Pure Shift NOESY and COSY. *Angewandte Chemie International Edition.* 51, 1-5, 2012.

Media:

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Staff:

- Industrial postdoc, Wangdong Ni (until 15/5 – 14) (L Nørgaard, Foss & R Bro)
- PhD student Klavs Martin Sørensen (until 31/5 – 15) (SB Engelsen)
- Industrial PhD student, Anna Klimkiewicz (until 30/7-15) (CB Zachariassen, Novozymes & Fvd Berg)

Guest Researchers:

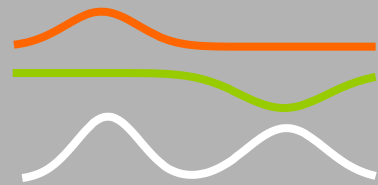
- Arantxa del Olmo Alvarez (host J Amigo, 1/3-15/7 – 2012)
- Carmen Estepa (host J Amigo, 18/4-10/7 – 2012)
- Silvia Grassi (host J Amigo, 30/4-31/10 – 2012)
- Candy Ruiz & Rosario Rojas Duran (host MA Petersen, 25/6 – 6/7-2012)

PhD defences:

- Morten Arendt Rasmussen (supervisor R Bro): MEDICOMETRICS. May 23rd 2012
- Minah Mosele (supervisor Å Hansen): Chemical and Structural Characterisation of Marama Bean (*Tylosema esculentum*) Carbohydrates. June 25th 2012

BSc & MSc defences:

- Claudia Been (supervisor R Bro): A multivariate approach to observational epidemiology. June 19th 2012
- Anna Klimkiewicz (supervisor SB Engelsen): Effective real-time evaluation of freshness of meat & fish samples for pet food. June 22nd 2012



Courses:

- Råvarekvalitet (Å Hansen & MA Petersen, 22 students, block 3)
- Thematic course – Integrated sensory and instrumental flavour research (MA Petersen, 30 students, block 4)
- Thematic course – Process Analytical Technology (T Skov, 3 students, block 3 & 4)
- Lectures and exercises in cool climate viticulture and enology (MA Petersen, block 4)
- PhD course – Advanced MATLAB (J Amigo, 10 students)
- PhD course – Introduction to R, MATLAB and Chemometrics (J Amigo, 12 students)
- PhD course – Quantitative Food Spectroscopy (N Viereck, 5 students, June)
- Odin course – Basic Chemometrics (MA Rasmussen, 15 students, April)
- CHANCE courses (J Amigo):
 - Advanced classification methods (April)
 - Analysis of descriptive sensory data by the use of PanelCheck (May)
 - Curve resolution in chemistry (June)

New granted projects:

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