

ISSUE 34 (JANUARY-MARCH 2013)



FOODOMICS: INTRODUCING ADVANCED QSPR METHODS FOR THE DEVELOPMENT OF HEALTHY EXTRUDED SNACKS FOR PROTEIN LIMITED POPULATIONS

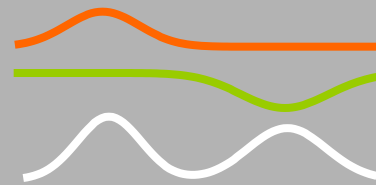
New Advanced Technology Foundation project to Q&T (Mette Hølse) in collaboration with the Fan Milk Group. The aim is to develop a prototype legume based extruded snack product targeted for protein limited populations by using Quantitative Structure-Property relationship methods

LIQFUN: DEVELOPMENT OF A LIQUID MATRIX WITH BETA-GLUCAN FIBRE FUNCTIONALITY

New Advanced Technology Foundation project to Q&T (Mette Skau Mikkelsen) in collaboration with Carlsberg. The primary success criteria for this project will be to demonstrate an optimal structure of β -glucan fibres where functionality is retained in a liquid beverage matrix



RASMUS BRO APPOINTED AS PROFESSOR EXTRAORDINARY AT UNIVERSITY OF STELLENBOSCH



Peer reviewed publications Jan-Mar 2013:

MM Løkke, HF Seefeldt, T Skov, M Edelenbos. Color and textural quality of packaged wild rocket measured by multispectral Imaging. *Postharvest Biology and Technology*. 75, 86–95, 2013.

C Varming, MA Petersen, T Skov, Y Ardö. Challenges in quantitative analysis of aroma compounds in cheeses with different fat content and maturity level. *International Dairy Journal*. 29 (1), 15-20, 2013.

D Raijada, AD Bond, FH Larsen, C Cornett, H Qu, J Rantanen. Exploring the Solid-Form Landscape of Pharmaceutical Hydrates: Transformation Pathways of the Sodium Naproxen Anhydrate-Hydrate System. *Pharmaceutical Research*. 30 (1), 280–289, 2013.

AA Gowen, JM Amigo, R Tsenkova. Characterisation of hydrogen bond perturbations in aqueous systems using aquaphotomics and multivariate curve resolution-alternating least squares. *Analytica Chimica Acta*. 759, 8-20, 2013.

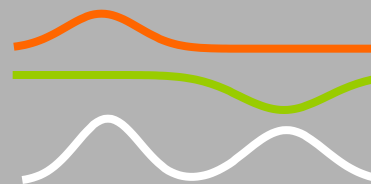
A Zira, S Kostidisa, S Theocharis, F Sigala, SB Engelsen, I Andreadou, E Mikros. ¹H NMR-based metabonomics approach in a rat model of acute liver injury and regeneration induced by CCl₄ administration. *Toxicology*. 303, 115-124, 2013.

SL Jensen, FJ Larsen, O Bandsholm, A Blennow. Stabilization of semi-solid-state starch by branching enzyme-assisted chain-transfer catalysis at extreme substrate concentration. *Biochemical Engineering Journal*. 72, 1-10, 2013.

C Varming, LT Andersen, MA Petersen, Y Ardö. Flavour compounds and sensory characteristics of cheese powders made from matured cheeses. *International Dairy Journal*. 30 (1), 19-28, 2013.

H Babamoradi, F van den Berg, Å Rinnan. Bootstrap based confidence limits in principal component analysis — A case study. *Chemometrics and Intelligent Laboratory Systems*. 120, 97–105, 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.



RW Adams, CM Holroyd, JA Aguilar, M Nilsson, GA Morris. “Perfecting” WATERGATE: Clean proton NMR spectra from aqueous solution. *Chemical Communications*. 49 (4), 358-360, 2013.

M Kristensen, F Savorani, S Christensen, SB Engelsen, S Bügel, S Toubro, I Tetens, A Astrup. Flaxseed dietary fibers suppress postprandial lipemia and appetite sensation in young men. *SciVerse ScienceDirect*. 23, 136-143, 2013.

H Pindstrup, C Fernández, JM Amigo, LH Skibsted. Multivariate curve resolution of spectral data for the pH-dependent reduction of ferrylmyoglobin by cysteine. *Chemometrics and Intelligent Laboratory Systems*. 122, 78–83, 2013.

R Bro, HJ Nielsen, F Savorani, K Kjeldahl, IJ Christensen, N Brüner, AJ Lawaetz. Data fusion in metabolomic cancer diagnostics. *Metabolomics*. 9 (1), 3–8, 2013.

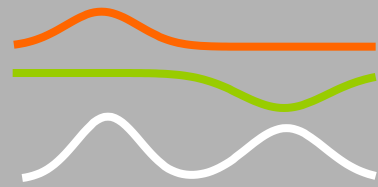
L Torri, C Dinnella, A Recchia, T Næs, H Tuorila, E Monteleone. Projective Mapping for interpreting wine aroma differences as perceived by naïve and experienced assessors. *Food Quality and Preference*. 29 (1), 6-15, 2013.

JX Wu, F van den Berg, SV Søgaard, J Rantanen. Fast-track to A Solid Dispersion Formulation Using Multi-way Analysis of Complex Interactions. *Journal of Pharmaceutical Sciences*. 102 (3), 904-914, 2013.

L Christensen, P Ertbjerg, H Løje, J Risbo, F van den Berg, M Christensen. Relationship between meat toughness and properties of connective tissue from cows and young bulls heat treated at low temperatures for prolonged times. *Meat Science*. 93 (4), 787-795, 2013.

S Hoff, J Damgaard, MA Petersen, BM Jespersen, ML Andersen, MN Lund. Influence of Barley Varieties on Wort Quality and Performance. *Journal of Agricultural and Food Chemistry*. 61 (8), 1968-1976, 2013.

S Hoff, FH Larsen, ML Andersen, MN Lund. Quantification of protein thiols using ThioGlo 1 fluorescent derivatives and HPLC separation. *Analyst*. 138 (7), 2096-2103, 2013.



A Birch, MA Petersen, ÅS Hansen. The aroma profile of wheat bread crumb influenced by yeast concentration and fermentation temperature. *LWT - Food Science and Technology*. 50 (2), 480-488, 2013.

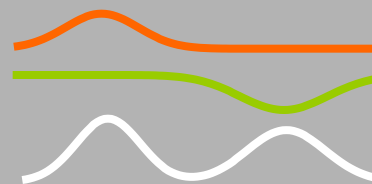
T Næs, E Monteleone, A Segtnan, M Hersleth. A comparison of two new take-away strategies and their relation to rating and ranking of extrinsic properties of dry cured ham. *Food Quality and Preference*. 27 (1), 63-71, 2013.

MS Mikkelsen, BM Jespersen, FH Larsen, A Blennow, SB Engelsen. Molecular structure of large-scale extracted β -glucan from barley and oat: Identification of a significantly changed block structure in a high β -glucan barley mutant. *Food Chemistry*. 136 (1), 130–138, 2013.

KM Sørensen, M Christensen, SB Engelsen. Three-dimensional images of porcine carcass fat quality using spatially resolved near infrared spectroscopy. *NIR News*. 24 (2), 9-10, 2013.

FJ McEvoy, JM Amigo. Using machine learning to classify image features from canine pelvic radiographs: Evaluation of partial least Squares discriminant analysis and artificial neural network models. *Vet Radiol Ultrasound*. 54 (2), 122-126, 2013.

S Warnecke, Å Rinnan, M Allesø, SB Engelsen. Measurement of active content in escitalopram tablets by a near-infrared transmission spectroscopy model that encompasses batch variability. *Journal of pharmaceutical Sciences*. 102 (4), 1268-1280, 2013.



Other publications:

SE Engelsen, R Bro, L Nørgaard. Multieksponentiel analyse: CuSO_4 , relaxometri og multivejskemometri. *Dansk Kemi. Det Kemometriske Rum.* 94, 1-2, 2013.

SE Engelsen, R Bro, L Nørgaard. Kalibrering med multivejsdata – teorien bag. *Dansk Kemi. Det Kemometriske Rum.* 94, 3, 2013.

T Skov, SB Engelsen. Chemometrics, mass spectrometry, and foodomics. In: *Foodomics: Advanced Mass Spectrometry in Modern Food Science and Nutrition.* Alejandro Cifuentes (red.). 507-538, 2013.

F Savorani, G Tomasi, SB Engelsen. Alignment of 1D NMR Data using the iCoshift tool: A Tutorial. In: *Magnetic Resonance in Food Science: Food for Thought.* John van Duynhoven (red.). 14-24. 2013.

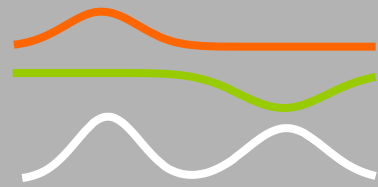
N Viereck, KM Sørensen, SB Engelsen. Investigating Depth Profiles from Porcine Adipose Tissue by HR MAS NMR Spectroscopy. In: *Magnetic Resonance in Food Science: Food for Thought.* John van Duynhoven (red.). 81-89, 2013.

Nuno Ratola, José Manuel Amigo, Sílvia Lacorte, Damià Barceló, Eleftheria Psillakis, Arminda Alves. Biomonitoring of Polycyclic Aromatic Hydrocarbons by Pine Needles: Levels and Trends in Southern Europe. In: *Handbook of Polycyclic Aromatic Hydrocarbons: Chemistry, Occurrence and Health Issues.* Guilherme C. Bandeira (red.). 83-114, 2013.

Media:

JM Amigo. Water, water: Aqueous perturbations. www.spectroscopynow.com. January 15th, 2013.

T Skov. Dansk biotek i nyt forskersamarbejde. *Politiken.* February 1st, 2013.



Staff:

- Age Smilde, external professor 20% (R Bro)
- Mette Skau Mikkelsen, post doc until 31/1 – 2014
- Carina Svendsen, PhD student until 31/3 – 2016 (T Skov/Fvd Berg)
- Carina Bruun Pedersen, lab trainee until 31/1 – 2014 (N Viereck)

Guest Researchers:

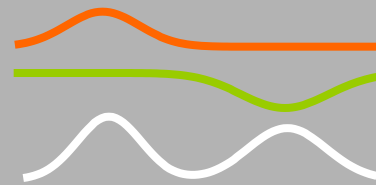
- Eva Borrás (host JM Amigo, 17/1-17/3 – 2013)
- Shanshan Cui (host ÅS Hansen, 18/2-19/8 – 2013)
- Marietta Kokla (host JM Amigo 18/2-18/8 – 2013)
- Eizo Taira (host JM Amigo 20/3-20/12 – 2013)

PhD defences:

- Mette Skau Mikkelsen (supervisor SB Engelsen): Comparison of functional and nutritional characteristics of barley and oat mixed linkage β -glucans. January 11th, 2013.
- Lea Giørtz (supervisor R Bro): Processing of chromatographic signals how to separate the wheat from the chaff. March 4th, 2013.

BSc & MSc defences:

- BSc: Søren Mellekjær Jensen (supervisor MA Rasmussen): Evaluation of suitable preprocessed techniques on NIR and IR spectroscopical data of 32 marzipan samples. February 15th, 2013.



Courses:

- Plant Polysaccharides (FH Larsen, SB Engelsen, 15 students, block 2)
- Advanced Chemometrics (R Bro, 12 students, block 2)
- Quantitative Bio-spectroscopy (N Viereck, FH Larsen, SB Engelsen, 16 students, block 2)
- Food Texture and Functionality (ÅS Hansen, 19 students, block 2)
- Brewing 1 (BM Jespersen, F van den Berg, 28 students, block 2)
- Råvarekvalitet (ÅS Hansen, BM Jespersen, MA Petersen, 90 students, block 3)
- Thematic Course: Process Analytical Technology (Fvd Berg, 7 students, block 3+4)
- Lectures in: Seed Science and Technology (BM Jespersen, block 2)
- Lectures in Advanced Sensory Methods and Sensometrics (T Skov, 26 students, block 3)
- Lectures in Analytical Chemistry (T Skov, 60 students, block 3)
- Lectures and exercises in: Food Enzymes and Applications (BM Jespersen, 22 students, block 3)
- Lectures in: Thematic Course: Dairy Processes and Equipment (Fvd Berg, 10 students, block 3)
- PhD: Preprocessing of quantitative NMR data for Chemometric Analysis (F Savorani, 7 students, block 3)
- ODIN: Basic Chemometrics (MA Rasmussen, 10 students, February)
- ODIN: Design of Experiments (Fvd Berg, 7 students, March)

New granted projects:

- Foodomics – Introducing advanced QSPR methods for the development of healthy extruded snacks for protein limited populations. Mette Hølse, Advanced Technology Foundation (3 years post doc; [see front page](#))
- LIQFUN – Development of a liquid matrix with beta-glucan fibre functionality. Mette Skau Mikkelsen, Advanced Technology Foundation (1 year post doc prolongation; [see front page](#))