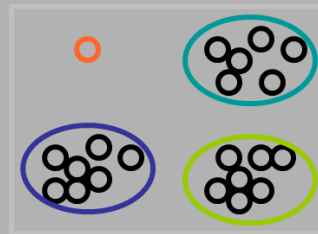


# SPECTROSCOPY & CHEMOMETRICS

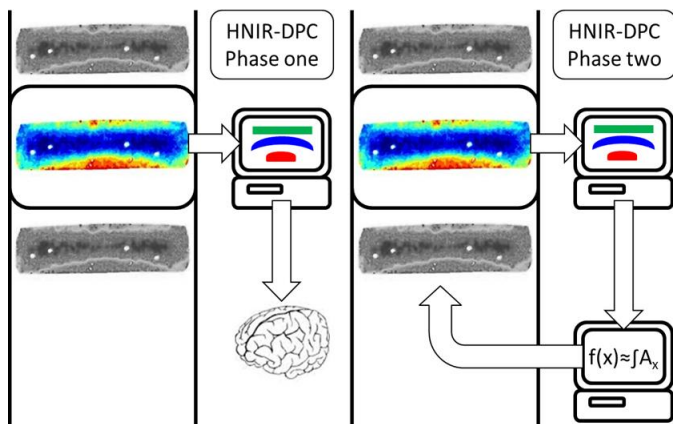
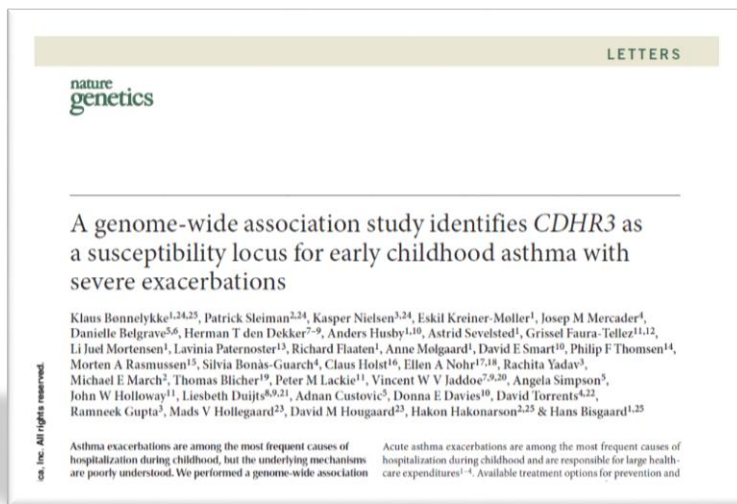


ISSUE 38 (JANUARY-MARCH 2014)

## FIRST NATURE PUBLICATION FROM DEPARTMENT OF FOOD SCIENCE BY SPECC PHD

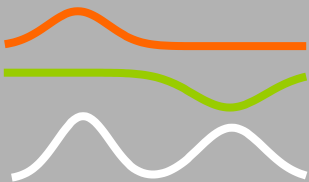
### MORTEN A. RASMUSSEN:

In collaboration with the Danish Pediatric Asthma Center at Copenhagen University Hospital in Gentofte and many others, SPECC PostDoc Morten A Rasmussen published in Nature Genetics on a GWAS study on early childhood asthma

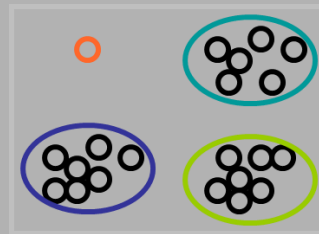


## NEW PROJECT WITH ARLA AMBA: HYPER SPECTRAL NEAR INFRARED IN DAIRY PROCESS CONTROL (HNIR-DPC)

The Advanced Technology Foundation and ARLA amba have rewarded SPECC PostDoc Hamid Babamoradi with a 2 mio DKK, two year, grant for the research project concerning the development of advanced automation of slicing, grating and packaging of cheeses.



# SPECTROSCOPY & CHEMOMETRICS



## Peer reviewed publications Jan-Mar 2014:

**I Endrizzi, F Gasperi, M Rødbotten, T Næs.** Interpretation, validation and segmentation of preference mapping models. *Food Quality and Preference*. 32, 198–209, 2014.

**T Næs, O Tomic, K Greiff, K Thyholt.** A comparison of methods for analyzing multivariate sensory data in designed experiments – A case study of salt reduction in liver paste. *Food Quality and Preference*. 33, 64–73, 2014.

**R Romano, C Davino, T Næs.** Classification trees in consumer studies for combining both product attributes and consumer preferences with additional consumer characteristics. *Food Quality and Preference*. 33, 27–36, 2014.

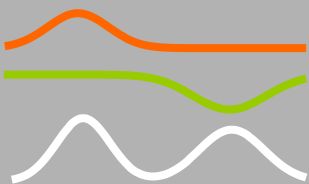
**L Louw, S Oelofse, T Næs, M Lambrechts, P van Rensburg, H Nieuwoudt.** Trained sensory panellists' response to product alcohol content in the projective mapping task: Observations on alcohol content, product complexity and prior knowledge. *Food Quality and Preference*. 34, 37–44, 2014.

**S Grassi, JM Amigo, CB Lyndgaard, R Foschino, E Casiraghi.** Beer fermentation: Monitoring of process parameters by FT-NIR and multivariate data analysis. *Food Chemistry*. 155, 279–286, 2014.

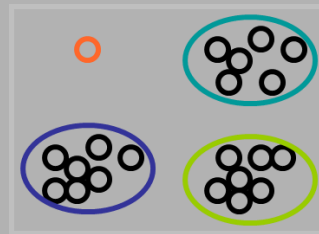
**E Borràs, JM Amigo, F van den Berg, R Boqué, O Busto.** Fast and robust discrimination of almonds (*Prunus amygdalus*) with respect to their bitterness by using near infrared and partial least squares-discriminant analysis. *Food Chemistry*. 153, 15–19, 2014.

**LG Johnsen, JM Amigo, T Skov, R Bro.** Automated resolution of overlapping peaks in chromatographic data. *Journal of Chemometrics*. 28 (2), 71–82, 2014.

**J Omar, M Olivares, JM Amigo, N Etxebarria.** Resolution of co-eluting compounds of *Cannabis Sativa* in comprehensive two-dimensional gas chromatography/mass spectrometry detection with Multivariate Curve Resolution-Alternating Least Squares. *Talanta*. 121, 273–280, 2014.



# SPECTROSCOPY & CHEMOMETRICS



## Peer reviewed publications Jan-Mar 2014:

**K Bønnelykke, P Sleiman, K Nielsen, E Kreiner-Møller, JM Mercader, D Belgrave, HT den Dekker, A Husby, A Sevelsted, G Faura-Tellez, LJ Mortensen, L Paternoster, R Flaaten, A Mølgaard, DE Smart, PF Thomsen, MA Rasmussen, S Bonàs-Guarch, C Holst, EA Nohr, R Yadav, ME March, T Blicher, PM Lackie, VWV Jaddoe, A Simpson, JW Holloway, L Duijts, A Custovic, DE Davies, D Torrents, R Gupta, MV Hollegaard, DM Hougaard, H Hakonarson, H Bisgaard.** A genome-wide association study identifies CDHR3 as a susceptibility locus for early childhood asthma with severe exacerbations. *Nature Genetics*. 46 (1), 51-58, 2014.

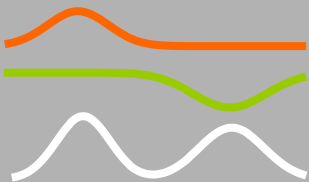
**JA Aguilar, RW Adams, M Nilsson, GA Morris.** Suppressing exchange effects in diffusion-ordered NMR spectroscopy. *Journal of Magnetic Resonance*. 238, 16–19, 2014.

**K Kjeldahl, MA Rasmussen, AL Hasselbalch, KO Kyvik, L Christiansen, S Rezzi, S Kochhar, TIA Sørensen, R Bro.** No genetic footprints of the fat mass and obesity associated (FTO) gene in human plasma <sup>1</sup>H CPMG NMR metabolic profiles. *Metabolomics*. 10 (1), 132–140, 2014.

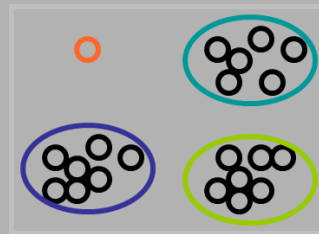
**KR Murphy, CA Stedmon, P Wenig, R Bro.** OpenFluor – an online spectral library of auto-fluorescence by organic compounds in the environment. *Analytical Methods*. 6 (3), 658–661, 2014.

**N Ratola, V Homem, JA Silva, R Araújo, JM Amigo, L Santos, A Alves.** Biomonitoring of pesticides by pine needles — Chemical scoring, risk of exposure, levels and trends. *Science of the Total Environment*. 476-477, 114–124, 2014.

**J Holm, LN Babol, N Markova, AJ Lawaetz, SI Hansen.** The interrelationship between ligand binding and thermal unfolding of the folate binding protein. The role of self-association and pH. *Biochimica et Biophysica Acta*. 1844 (3), 512–519, 2014.



# SPECTROSCOPY & CHEMOMETRICS



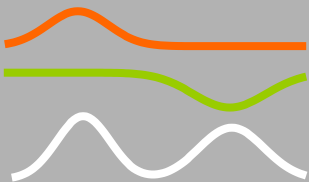
## Other publications Jan-Mar 2014:

**C Varming, JM Amigo, MA Petersen, T Toldam-Andersen.** Aroma Analysis and Data Handling in the Evaluation of Niche Apple Juices from 160 Local Danish Apple Cultivars. In: *Flavour Science: Proceedings from XIII Weurman Flavour Research Symposium*. Chapter 53, 277-281, 2014.

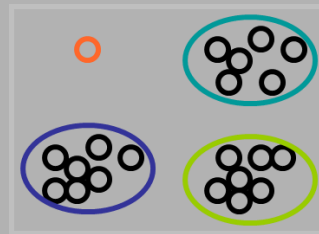
**Å Rinnan, JM Amigo, T Skov.** Multiway methods in food science. In: *Mathematical and Statistical Methods in Food Science and Technology*. Chapter 9, 143-174, 2014.

## Media:

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# SPECTROSCOPY & CHEMOMETRICS



## Staff:

- Susanne W Bruun, post doc 7/3 2014 – 31/12 2014 (Å Rinnan)
- Hamid Babamoradi, Industrial post doc 1/3 2014 – 29/2 2016 (JM Amigo)
- Christine Poulsen, MSc student 17/2 2014 – 15/8 2014 (N Viereck, K Sørensen, T Skov)
- Maria Tougaard Andersen, MSc student 17/2 2014 – 15/8 2014 (N Viereck, K Sørensen, T Skov)
- Jesper Kailow Hejselbæk, MSc student 24/2 2014 – 8/10 2014 (R Bro)

## Guest Researchers:

- Raffaele Civelli (host JM Amigo, 1/2 – 31/5 2014)
- Sofia Tirado Santos (host JM Amigo, 5/2 – 30/6 2014)
- Guilherme Alexandrino (host JM Amigo, 5/2 – 31/8 2014)
- MSc stud Sara Mesquita, (host Å Rinnan, 10/2 – 15/7 2014)

## PhD defences:

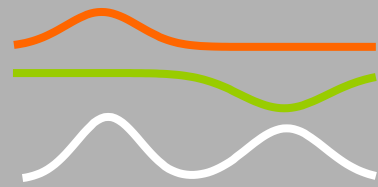
- **Solveig Warnecke** (supervisor Å Rinnan): New PAT tools for assessing content uniformity, sampling error, and degree of crystallinity in pharmaceutical tablets. January 6<sup>th</sup>, 2014
- **Karin Kjeldahl** (supervisor R Bro): Towards improved biomarker research - Data analytical challenges of high-dimensional biological data. February 5<sup>th</sup>, 2014

## BSc & MSc defences:

- Margrethe Le Thuy Nhi Hoang, BSc (supervisor FH Larsen): Forskellige bryggetider og temperaturers indflydelse på indholdsstoffer i grøn og sort te. January 24<sup>th</sup>, 2014
- Maina Abbasi, BSc (supervisor FH Larsen): Analysis of coffee by nuclear magnetic resonance (NMR) spectroscopy and gas chromatography-mass spectrometry (GC-MS). March 7<sup>th</sup>, 2014
- Katrine Byriel Bjørn, MSc (supervisor Å Rinnan): Variations and deviations in nutrient composition of total and partly mixed rations for dairy cows. March 18<sup>th</sup>, 2014



# Spectroscopy & Chemometrics



## **Courses Jan – Mar:**

### **Block 3:**

- Food Process Equipment (F van den Berg, 44 students)
- Lectures in: Advanced Sensory Methods and Sensometrics (Å Rinnan, 50 students)
- Lecture in: Brewing 2 (F van den Berg)
- PhD: Preprocessing of quantitative NMR data for Chemometric Analysis (F Savorani, 10 students)
- ODIN: PanelCheck for analyzing sensory profiling data, 4/2 – 2014
- ODIN: Basic Chemometrics, 5-6/3 – 2014

### **New granted projects:**

- HNIR-DPC – Hyperspectral Near Infrared in Dairy Process Control. Hamid Babamoradi, Advanced Technology Foundation (2 years post doc)