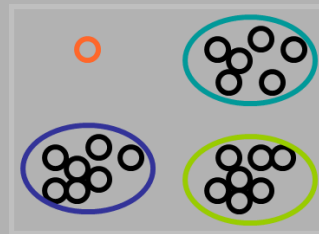


# SPECTROSCOPY & CHEMOMETRICS



ISSUE 39 (APRIL-JUNE 2014)

## SPECC ASSOCIATE THOMAS SKOV RECEIVES THE RESEARCHER PRIZE FROM HRH THE PRINCE CONSORT'S FOUNDATION"

Thomas receives the 2014 HRH award for his research as well as to extend the use of chemometrics in an industrial context

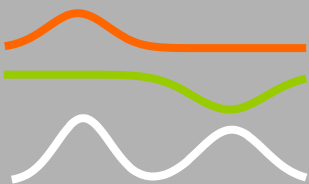


## SPECC ASSOCIATE JOSÉ MANUEL AMIGO RECEIVES A PRESTIGIOUS CHEMOMETRICS AWARD:

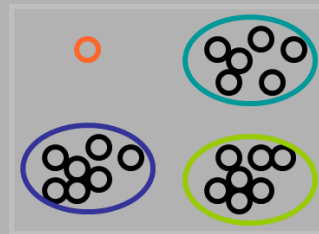
José receives the 2014 Chemometrics and Intelligent Laboratory Systems Award due to his significant contribution to the development and dissemination of chemometrics worldwide

**NEW PROJECT WITH CHR. HANSEN A/S: PLANTEPIGMENT**  
SPECC associate Åsmund Rinnan is involved in a large GUDP project together with Chr. Hansen A/S concerning the development of plants for the production of natural colorants for food





# SPECTROSCOPY & CHEMOMETRICS



## Peer reviewed publications Apr-Jun 2014:

**E Menichelli, T Almøy, O Tomic, NV Olsen, T Næs.** SO-PLS as an exploratory tool for path modelling. *Food Quality and Preference*. 36, 122–134, 2014.

**S Grassi, JM Amigo, CB Lyndgaard, R Foschino, E Casiraghi.** Assessment of the sugars and ethanol development in beer fermentation with FT-IR and multivariate curve resolution models. *Food Research International*. 62, 602–608, 2014.

**S Grassi, C Alamprese, V Bono, E Casiraghi, JM Amigo.** Modelling Milk Lactic Acid Fermentation Using Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS). *Food Bioprocess Technol*. 7, 1819–1829, 2014.

**L Lenhardt, I Zekovic, T Dramicanin, MD Dramicanin, R Bro.** Determination of the Botanical Origin of Honey by Front- Face Synchronous Fluorescence Spectroscopy. *Applied Spectroscopy*. 68 (5), 557-563, 2014.

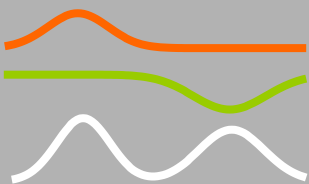
**K Sulek, LK Vigsnaes, LR Schmidt, J Holck, HL Frandsen, J Smedsgaard, T Skov, AS Meyer, TR Licht.** A combined metabolomic and phylogenetic study reveals putatively prebiotic effects of high molecular weight arabino-oligosaccharides when assessed by in vitro fermentation in bacterial communities derived from humans. *Anaerobe*. 28, 68-77, 2014.

**M-B Gholivand, R Jalalvand, HC Coicochea, T Skov.** Chemometrics-assisted simultaneous voltammetric determination of ascorbic acid, uric acid, dopamine and nitrite: application of non-bilinear voltammetric data for exploiting first-order advantage. *Talanta*. 119, 553-563, 2014.

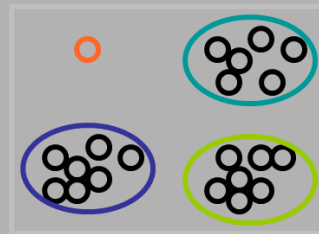
**A Bergström, T Skov, MI Bahl, HM Roager, LB Christensen, KT Ejlerskov, C Mølgaard, KF Michaelsen, TR Licht.** Establishment of Intestinal Microbiota during Early Life: a Longitudinal, Explorative Study of a Large Cohort of Danish Infants. *Applied and Environmental Microbiology*. 80 (9), 2889–2900, 2014.

**Å Rinnan.** Pre-processing in vibrational spectroscopy – when, why and how. *Analytical Methods (Online)*. 1-6, 2014.

**MÁ Fernández de la Ossa, C García-Ruiza, JM Amigo.** Near promising future of near infrared hyperspectral imaging in forensic sciences. *NIRnews*. 25 (4), 6-9, 2014.



# SPECTROSCOPY & CHEMOMETRICS



## Peer reviewed publications Apr-Jun 2014:

**M-B Gholivand, AR Jalalvand, HC Goicoechea, T Skov.** Fabrication of an ultrasensitive impedimetric buprenorphine hydrochloride biosensor from computational and experimental angles. *Talanta*. 124, 27–35, 2014.

**HM Roager, K Sulek, K Skov, HL Frandsen, J Smedsgaard, A Wilcks, T Skov, SG Villas-Boas, TR Licht.** Lactobacillus acidophilus NCFM affects vitamin E acetate metabolism and intestinal bile acid signature in monocolonized mice. *Gut Microbes*. 5 (3), 1-8, 2014.

**JM Larsen, S Brix, AH Thyssen, S Birch, MA Rasmussen, H Bisgaard.** Children with asthma by school age display aberrant immune responses to pathogenic airway bacteria as infants. *Journal of Allergy and Clinical Immunology*. 133 (4), 1008–1013, 2014.

**MM Vega, C Varming, T Skov, TB Toldam-Andersen.** Post-harvest ripening increase cultivar specific sensory and analytical aroma profile in apple juice: A study of four commercial cultivars in Denmark. *Acta Agriculturae Scandinavica, Section B – Soil & Plant Science*. 64 (3), 244–251, 2014.

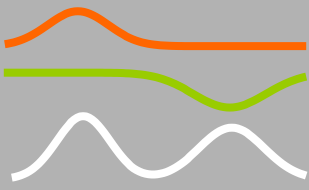
**R Bro, AK. Smilde.** Principal component analysis. *Analytical Methods*. 6, 2812–2831, 2014.

**MA Rasmussen, E Maslova, TI Halldorsson, SF Olsen.** Characterization of Dietary Patterns in the Danish National Birth Cohort in Relation to Preterm Birth. *PLOS ONE*. 9 (4), 1-9, 2014.

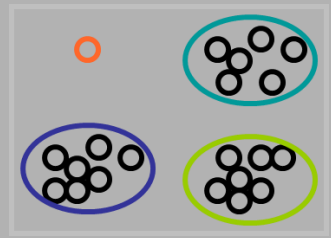
**CB Lyndgaard, MA Rasmussen, SB Engelsen, D Thaysen, F van den Berg.** Moving from recipe-driven to measurement-based cleaning procedures: Monitoring the Cleaning-In-Place process of whey filtration units by ultraviolet spectroscopy and chemometrics. *Journal of Food Engineering*. 126, 82–88, 2014.

**SB Engelsen, PI Hansen, S Pérez.** POLYS 2.0: An Open Source Software Package for Building Three-Dimensional Structures of Polysaccharides. *Biopolymers*. 101 (7), 733-743, 2014.

**Å Rinnan, M Andersson, C Ridder, SB Engelsen.** Recursive weighted partial least squares (rPLS): an efficient variable selection method using PLS. *Journal of Chemometrics*. 28, 439–447, 2014.



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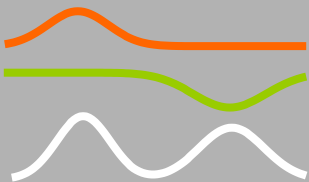
## Other publications Apr-Jun 2014:

**E Garcia, K König, I Klaas, JM Amigo, BH Allesen-Holm, R Bro, C Enevoldsen.**

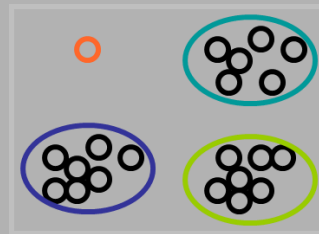
Detecção de claudicação – o reconhecimento de padrões em dados de sistema de ordenha robótica e os desafios em classificar o grau de claudicação. *CIÊNCIAS VETERINÁRIAS: PRAXIS E FUTURO*. 3-5 de abril, 2014.

**Media:**

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# SPECTROSCOPY & CHEMOMETRICS



## Staff:

- Charlotte Amalie Juul Pedersen, MSc student 7/4 2014 – 1/1 2015 (F van den Berg)
- Chang Liu, MSc student 2/6 2014 – 2/3 2015 (FH Larsen)
- Signe Maria Udengaard Christensen, MSc student 2/6 2014 – 15/4 2015 (Å Rinnan)
- Peter Bæk Skou, MSc student 16/6 – 18/8 2014 (R Bro)
- Esben Bjerrum, post doc 1/6 – 31/12 2014 (T Skov)
- Maj-Britt Schmidt Andersen, post doc 1/4 2014 – 1/4 2015 (Å Rinnan)

## Guest Researchers:

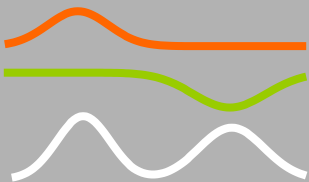
- Javier Escudero (host E Acar, 16/6 – 18/7 2014)
- Engin Cukuroglu (host E Acar, 16/6 – 15/8 2014)
- Ebenezer De Oliveira Silva (host Å Rinnan, 16/6 – 1/7 2014)
- Alper Baspinar (host E Acar, 16/6 – 15/8 2014)
- Martyna Jackowska (host JM Amigo, 13/6 – 18/7 2014)
- Jose Martin Ramos Diaz (host Å Rinnan, 1/5 – 30/6 2014)

## PhD defences:

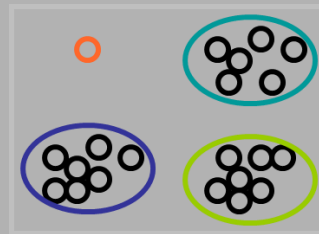
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## BSc & MSc defences:

- Marie Wolsing, MSc (supervisor F van den Berg): Online spectroscopy in flow chemistry. June 20<sup>th</sup>, 2014
- Katharina Böckmann, MSc (supervisor F van den Berg): Quantification of API in intravaginal rings by Raman and analysis of their engineering and release profile. June 17<sup>th</sup>, 2014



# SPECTROSCOPY & CHEMOMETRICS



## Courses Apr – June

### Block 4:

- Process Analytical Chemistry and Technology (F van den Berg and T Skov, 10 students)
- Lecture in: Thematic course: Integrated Sensory and Instrumental Flavour Research (T Skov, 28 students)
- PhD: Introduction to MATLAB for Multivariate Data Analysis (18 students, JM Amigo)
- PhD: Advanced MATLAB for Multivariate Data Analysis (19 students, JM Amigo)
- PhD: Copenhagen School of Chemometrics – CSC (16/6 – 18/7. 23 students, JM Amigo)

### New granted projects:

- PlantePigment - the development of plants for the production of natural colorants for food. Åsmund Rinnan, GUDP (2014-2017)