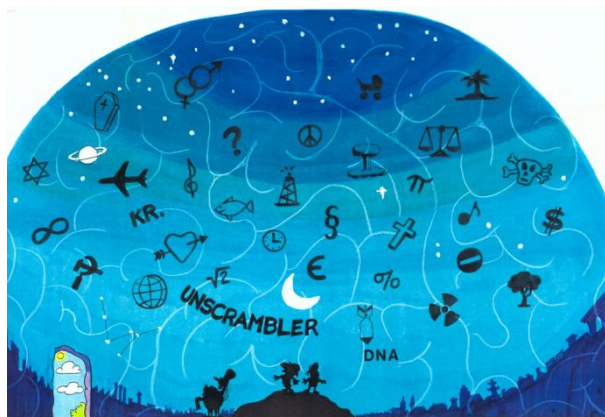


ISSUE 22 (JAN-MARCH)



BRAIN FOR A NIGHT

Congratulations to Q&T PhD student **Signe Hoff** who was awarded “Brain for a Night” at KU-LIFE for a presentation of her MSc work. Beside the honor she also received 10.000 DKK

Q&T IN CHARGE OF TWO FACULTY ELITE RESEARCH AREAS

Chemometrics, biostatistics and multivariate dataanalysis (**Rasmus Bro**)
Metabolomics and bioactive substances (**Søren Balling Engelsen**)

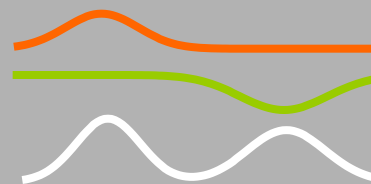
Peer-reviewed publications

M Alvarez-Guerra, D Ballabio, JM Amigo, R Bro, JR Viguri. Development of models for predicting toxicity from sediment chemistry by partial least squares-discriminant analysis and counter-propagation artificial neural networks. *Environmental Pollution* **158: 607–614, 2010**

M Vidal, JM Amigo, R Bro, M Ostra and C Ubide. Quantitative determination of additives in a commercial electroplating nickel bath by spectrophotometry and multivariate analysis. *Analytical Methods* **2: 86–92, 2010**

N Ratola, JM Amigo and A Alves. Levels and sources of PAHs in selected sites from Portugal: Biomonitoring with *Pinus pinea* and *Pinus pinaster* needles. *Arch Environ Contam Toxicol* **58:631–647, 2010**

M Kristensen, F Savorani, G Ravn-Haren, M Poulsen, J Markowski, FH Larsen, LO Dragsted and SB Engelsen. NMR and interval PLS as reliable methods for determination of cholesterol in rodent lipoprotein fractions. *Metabolomics* **6:129–136, 2010**



S Bruun, JW Jensen, J Magid, J Lindedam and SB Engelsen. Prediction of the degradability and ash content of wheat straw from different cultivars using near infrared spectroscopy. *Industrial Crops and Products* **31: 321–326, 2010**

K Klausen, AG Mortensen, B Laursen, KF Haselmann, BM Jespersen and IS Fomsgaard. Phenolic compounds in different barley varieties: Identification by Tandem Mass Spectrometry (QStar) and NMR; Quantification by Liquid Chromatography Triple Quadrupole-Linear Ion Trap Mass Spectrometry (Q-Trap). *Natural Product Communications* **5 (3): 407-414, 2010**

CL Hansen, Å Rinnan, SB Engelsen, T Janhøj, E Micklander, U Andersen and FVD Berg. Effect of Gel Firmness at Cutting Time, pH, and Temperature on Rennet Coagulation and Syneresis: An in situ ^1H NMR Relaxation Study. *J. Agric. Food Chem.* **58: 513–519, 2010**

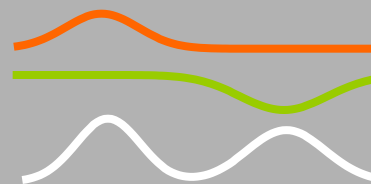
Å Rinnan, NJ Christensen and SB Engelsen. How the energy evaluation method used in the geometry optimization step affect the quality of the subsequent QSAR/QSPR models. *J Comput Aided Mol Des* **24:17–22, 2010**

F Savorani, G Picone, A Badiani, P Fagioli, F Capozzi and SB Engelsen. Metabolic profiling and aquaculture differentiation of gilthead sea bream by ^1H NMR metabonomics. *Food Chemistry* **120: 907–914, 2010**

F Savorani, G Tomasi and SB Engelsen. *Icoshift*. A versatile tool for the rapid alignment of 1D NMR spectra. *Journal of Magnetic Resonance* **202: 190–202, 2010**

NJ Christensen, PI Hansen, FH Larsen, T Folkerman, MS Motawia and SB Engelsen. A combined nuclear magnetic resonance and molecular dynamics study of the two structural motifs for mixed-linkage β -glucans: methyl β -cellobioside and methyl β laminarabioside. *Carbohydrate Research* **345: 474–486, 2010**

R Bro, N Viereck, M Toft, H Toft, PI Hansen and SB Engelsen. Mathematical chromatography solves the cocktail party effect in mixtures using 2D spectra and PARAFAC. *Trends in Analytical Chemistry* **29(4): 281-284, 2010**



Other Publications

R Bro, L Nørgaard and SB Engelsen, Det Kemometriske Rum – Ud med skidtet – behold kanelet: variabel-selektion, *Dansk Kemi*, **91(3): 28-29, 2010**

L Nørgaard, SB Engelsen and R Bro, Det Kemometriske Rum – Hvis fit er godt, hvad er overfit så?, *Dansk Kemi*, **91(1-2): 28-29, 2010**

E Skibsted and SB Engelsen. Spectroscopy for Process Analytical Technology (PAT). In: (J Lindon, G Tranter and D Koppenaal, ed.) Encyclopedia of Spectroscopy and Spectrometry, 2nd edition, Vol 3. Oxford: Elsevier; pp. 2651–2661, **2010**

Media

Birger Pedersen. Muligt kvantespring i cancer-diagnostik. Videnskab dk,

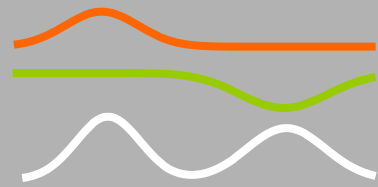
<http://videnskab.dk/composite-3875.htm>, 19. februar 2010

Staff:

- **Christina Aunsbak** (Feb 10 – Jan 11) - lab trainee
- **Gleb Dudnik** (Feb 10 – Jan 11) - lab trainee (stopped April)
- **Morten Arendt Rasmussen** in USA Jan - May 2010
- **Hanne Winning** return from maternity leave 15/2 2010
- **Mette Holse** return from South Africa 1/2 2010
- **Thomas Skov** return from South Africa 1/2 2010
- **Jonas Thygesen** in USA Mar – Aug 2010
- **Kristian Jørgensen** (Feb - Apr)
- **Åsmund Rinnan** is on paternity leave
- **Karin Kjeldahl** is on maternity leave
- **Mette Skau Nielsen** is on maternity leave
- **Anja Niehues** is on maternity leave

Guest Researchers:

- **Giuditta Marzorati** (SBE, FS, NV, Bachelor → June 25; IR and NMR spatially resolved spectroscopic measurements of fat from belly cuts of pigs)
- **Eleftheria Kakagianni** (SBE, NV, Bachelor → July 15; NMR spectroscopy of doped athletes)



Courses:

- Quantitative Food Spectroscopy – Block 2. 13 Participants. F H Larsen, S B Engelsen & N Viereck
- Råvarekvalitet (Quality of Raw Products) – Block 3 – 36 participants. Major contributor: Å Hansen
- Open House Q&T for future MSc students Friday March 26th 2010 (BMJ and RB)
- Process Analytical Technology – Block 3+4, 4 students (THSK)
- ODIN, Basic Chemometrics, 20 participants (THSK)
- ODIN, Design of experiments, 10 participants (FB)
- ODIN, Advanced Chemometrics 23-24 March, 7 participants (RB)
- ODIN, Process Spectroscopy/Chromatography workshop, 25 participants (THSK)