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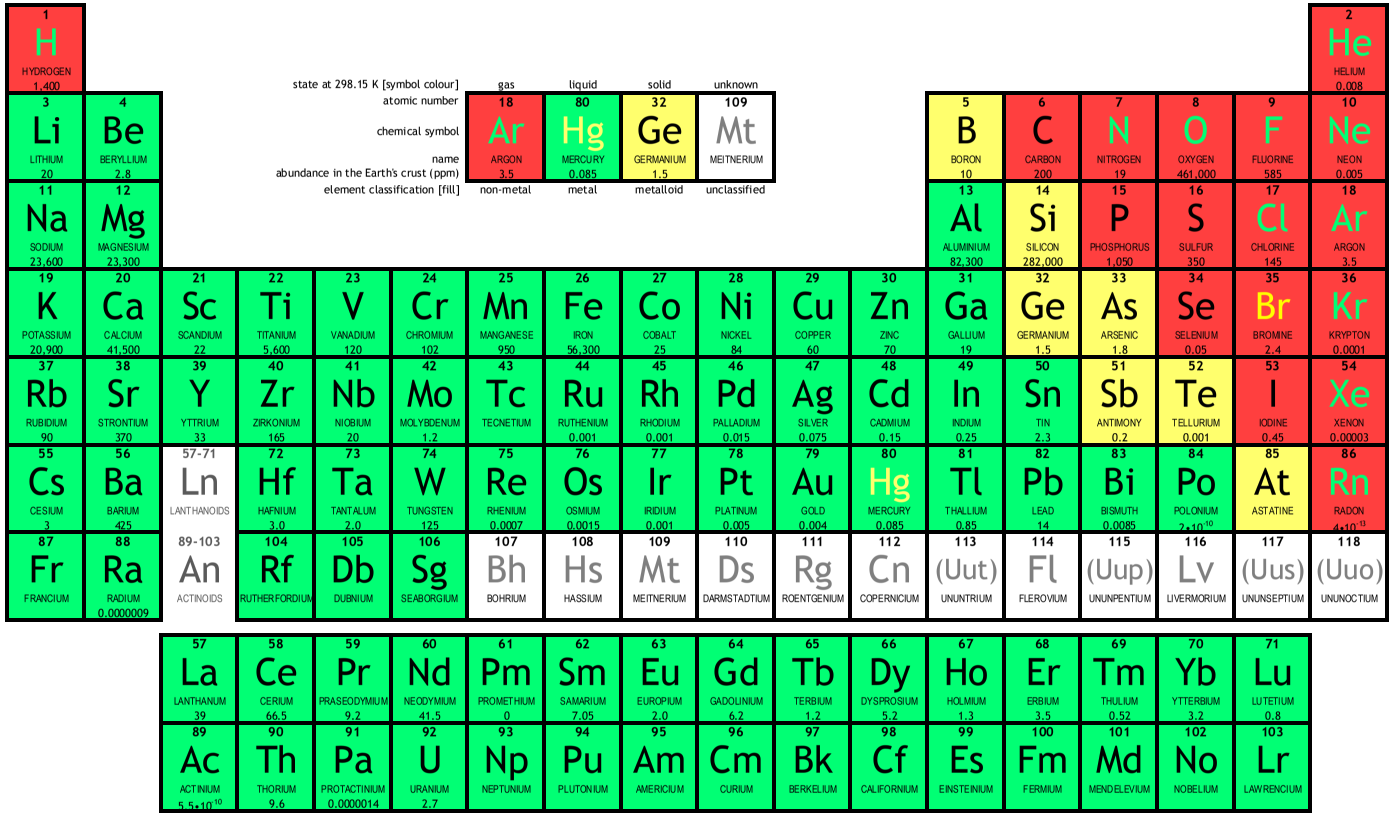
The Chemical Side of SLU^{2+}

Book of Abstracts

Edited by Daniel Lundberg

The Periodic Table of Elements



Welcome to the Chemical Side of SLU^{2+}!

In December 2008, the United Nations decided that 2011 would be the International Year of Chemisty with the theme *Chemistry – our life, our future*, focussing on the achievements of chemistry and its contributions to the well-being of mankind. Celebrations took place all over the world, often organized by the local or national chemistry community. Here, at SLU Uppsala, the previously existing Department of Chemistry arranged the first installment of the Chemical Side of SLU which included more than 70 participants, including 14 oral presentations and 38 posters.

Today, three years later, the department has reformed and also changed its name, two new chemical elements have been named, the United Nations has declared 2014 the International Year of Crystallography, *and* it is time for another edition of this symposium series: the Chemical Side of SLU^{2+}! Unlike the United Nations, however, we have chosen not to devote the entire symposium to crystallography, but rather again see chemistry as the wide area of study it is. This is reflected in this book of abstracts as researchers on our campuses study the chemistry of metabolites, bioactive molecules, nanomaterials, soils, pesticides, and – the focus of this "chemical" year – crystals.

We hope that this lunch-day-lunch symposium will result in many new contacts, the re-establishment and development of existing ones, as well as offering everyone an insight into what is happening in neighbouring areas at their home university – once again on the chemical side of SLU. Welcome!

The organizing committee
Uppsala, August 2014

Session 1

Soil, Environment, Speciation

"Judging by the pollution content of the atmosphere,
I believe we have arrived at the latter half of the 20th Century."

Capt. Spock
Star Trek IV: the Voyage Home

SES - Plenary

Interphase chemistry and geochemistry: what have we learned in the last 30 years

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Chemical reactions at mineral-aqueous solution interfaces have long been known to play a major role in determining the chemistry of the natural environment. From the 1940's to the present, there have been thousands of published studies of the sorption of inorganic and organic species at solid-water interfaces using adsorption isotherm methods.[1] While these studies provided valuable macroscopic information about the chemical reactivity of solid surfaces as well as K_D values for cation and anion removal from aqueous solutions, they did not provide the molecular-level details required to understand adsorption mechanisms and to distinguish between true adsorption and formation of solid precipitates.

Fast-forwarding to the late 1970's, some of the first IR spectroscopy studies of the interaction of organic bases and phosphate oxoanions with hydrous oxide surfaces were carried out by Parfitt et al.[2] In the mid-1980's, synchrotron-based X-ray absorption fine structure (XAFS) spectroscopy allowed us to extend these earlier spectroscopic studies to most cation and anion sorption products at mineral-water interfaces.[3]

Since those first XAFS experiments, there have been over 1,000 published XAFS spectroscopy studies of the molecular-level details of sorption complexes at solid-aqueous solution interfaces. I will review some of these studies, including several from my research group, which have focused on the interaction of aqueous metal ions with hydrated mineral surfaces, bacterial surfaces, biofilm-coated mineral surfaces, mineral surfaces coated with simple carboxylic acid molecules and natural organic matter, and natural and engineered nanoparticles. I will also review some of the results of other synchrotron-based methods used in interface chemistry studies such as soft X-ray photoemission, long-period X-ray standing wave fluorescence yield spectroscopy, resonant anomalous X-ray reflectivity, and crystal truncation rod diffraction, as well as non-synchrotron methods such as scanning probe microscopy, attenuated total reflectance FTIR spectroscopy, and photoacoustic spectroscopy, focusing on some of the things we have learned about interface chemistry and geochemistry over the past 30 years and what we do not know about the mineral-water interface.

[1] I. Cornet, *J. Chem. Phys.* **1943**, *11*, 217-226.
[2] Parfitt *J. Soil Sci.* **1977**, *28*, 29-39.
[3] Hayes et al., *Science* **1987**, *238*, 783-786.

Molybdenum binding to soil constituents in spodosols – an EXAFS and modelling study

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Molybdenum is a trace element with an important role in the biogeochemical cycle of nitrogen, as it is required for nitrogen fixation. Under conditions typical for podzols, dissolved molybdenum is expected to exist primarily as dissolved molybdate ions. Previous batch experiments have shown that molybdate is bound strongly at low pH in both organic horizons and in B horizons, indicating the involvement of both organic matter and iron/aluminium (hydr)oxides in the binding.

The purpose of this study was to obtain improved knowledge of the binding mechanisms, so that geochemical models can be set up to simulate the bioavailability and mobility of molybdenum under different conditions. To this end the coordination of added molybdate was studied by means of Mo *K*-edge EXAFS spectroscopy at the Stanford Synchrotron Radiation Lightsource (SSRL) beamline 4-1, for both model sorbents (ferrihydrite, aluminium hydroxide, Suwannee River fulvic acid) and natural soil samples (a mor layer and a podzol Bs horizon from Storå, central Sweden).

In summary, the spectroscopic results confirm that molybdate is bound to both organic matter and (hydr)oxides in soils.

Vanadium bioavailability in slag amended soils

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Ferrous blast furnace (BF) slags are by-products formed during the making of pig iron. Due to the alkalinity and physical properties of the BF slags they can be further used as soil amendments or applied in road materials and cement. Swedish BF slags are naturally high in vanadium which is of environmental concern as vanadium is readily toxic to plants. In this study, vanadium availability to barley was tested for two commercially available Swedish BF slags which contained 800 mg V kg^{-1}. The slags were applied at different doses to two soils in which barley shoot growth was evaluated. In addition, the soils were also treated with different concentrations of dissolved vanadate(V) and barley shoot growth was tested two weeks (freshly spiked) and 11 months (aged) after spiking. Vanadium speciation in the BF slags was investigated by XANES spectroscopy, showing that vanadium(II) and vanadium(III) were the dominating valence states. The most toxic vanadium form, vanadate(V), was however the main redox species expected in the soil solution. The BF slags did not significantly affect barley growth. In the BF slag amended soils, the bioavailable vanadium was controlled by leaching.

SES - Oral 3

Chromium(III) and bismuth(III) complexation to organic matter: EXAFS and equilibrium modelling

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The complexation of chromium(III) and bismuth(III) ions to organic matter was investigated by batch equilibrations with Suwannee River fulvic acid (SRFA) and with mor layer material (Risbergshöjden Oe). In the SRFA systems, 3 mM chromium(III) solutions were equilibrated with 9 $g \cdot l^{-1}$ SRFA and equilibrated at different pH values ranging from 2 to 6. The results show that chromium(III) formed monomeric organic complexes with SRFA. There was no evidence of polymerization with the exception of the particulate phase at pH 6, which was attributed to a limited extent of $Cr(OH)_3$ formation.

The experiments showed a predominance of monomeric organic complexes for chromium(III), with a dimeric complex formed at pH >5. The sorption of chromium(III) ions was pH dependent and to some extent influenced by competition from aluminium(III) and copper(II) ions. Chromium(III) complexation was found to be very slow at pH <4, and equilibration times of 3 months or longer were required to reach equilibrium under these conditions. The complexation of bismuth(III) remained essentially unchanged.

Removal of arsenic from drinking water

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Arsenic containing drinking water is major health problem in many parts of the world and the limit for arsenic concentration is set as low as 10 mg/dm^3 by WHO.[1] It is thus of utmost importance to develop methods to efficiently remove arsenic from drinking water at a low cost applicable in remote areas without access to electricity or educated personal.

This study shows that it is possible to remove arsenic from water independent of speciation by letting arsenic-enriched water pass a column of ferrihydrite-coated grains of sand or the commercial material, granular ferric hydroxide, GFH®.[2] Adsorption of considerable amounts of arsenate and arsenite were achieved on a sub-minute time scale with both adsorbents. Furthermore, efficient adsorption on GFH® can be achieved in seconds of empty bed contact time. Arsenate adsorption was affected by moderate changes in pH, while such an effect was negligible for arsenite. At slightly acidic pH substantially higher amounts of arsenate could be adsorbed. The iron content of the coated sand was varied and it was found that more arsenic was adsorbed on grains with a higher iron content, however, the relationship was far from proportional.

[1] *Guidelines for Drinking-Water Quality*, 2nd ed. WHO, **1993**.
[2] J. Mähler & I. Persson, *Appl. Geochem.* **2013**, *37*, 179-189.

SES - Oral 4

Differential fluorescence used to describe treatability of DOM during drinking water production

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Fluorescence spectroscopy has been widely used to characterize fluorescent dissolved organic matter (FDOM) in various waters including during drinking water production. In our study, samples were collected from four large water treatment plants in Sweden and analyzed for 3D fluorescence, absorbance and dissolved organic carbon. Our results show that chemical flocculation is selective towards FDOM with red-shifted emission across the entire EEM. The biological process of slow sand filtration was complementing to flocculation with targeted removal of FDOM with blue-shifted emission. Rank correlation showed that FDOM with red-shifted emission is coupled to chemical formulas with relatively high oxygen to carbon ratio rich in double bonds while FDOM with blue-shifted emission correlates with more aliphatic components with lower oxygen content.

Fifty years of monitoring of Swedish surface water chemistry

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For more than half a century, scientific insights from surface water monitoring have been a vital part of evidence-based environmental management in Sweden. Efforts to understand and control eutrophication in the 1960s resulted in the construction of waste water treatment plants with phosphorus precipitation, while acid rain research in the 1970s contributed to legislation curbing sulfur and nitrogen emissions. By the 1990s, relatively long time series data were being used to infer effects of climate variability and change on surface water chemistry.

Monitoring data play a key role in European water quality standards such as the Water Framework Directive and have been used to show the beneficial effects of agricultural management on nutrient loads and eutrophication of the Baltic Sea. The Swedish experience demonstrates that a well-designed and financially supported surface water monitoring program can be used to understand and manage a range of stressors and societal concerns. During the fifty year period, the contribution of one department, today the Department of Aquatic Sciences & Assessment at SLU, has ensured the high continuity of the monitoring.

Session 2

Biomaterials, Nano- & Biotechnology

"We are the Borg. Lower your shields and surrender your ships. We will add your biological and technological distinctiveness to our own. Your culture will adapt to service us. Resistance is futile."

The Borg Collective
Star Trek: First Contact

Nanocellulose: properties and applications

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&
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Cellulose is the most abundant polymer on earth and has a highly hierarchical structure. Nanocellulose is the product of cellulose fiber defibrillation into units featuring nanosize dimensions. Today, it is the sixth most investigated nanomaterial after carbon nanotubes, graphene, fullerenes, nanosilver, and nanotitania. Nanocellulose can be obtained from various sources including higher plants, algae, bacteria, fungi, and tunicates. Nanocellulose is a collective term for a family of heterogenous cellulosic nanomaterials, which differ greatly depending on their origin, processing, surface chemistry, charge, dimensions, and aspect ratio.

Thanks to its nanoenabled properties and high surface to volume ratio, nanocellulose features properties, which are different from those of cellulose fibers on macroscale. For instance, rheological, mechanical, optical, and magnetic properties of nanocellulose are very different from ordinary native cellulose. These properties are currently utilized in a number of application including mechanically strong lightweight materials, thermal and acoustic insulators, packaging and paper materials, paper-based energy storage devices, virus removal filters, and materials for medicinal use.

Molecular mechanisms of spider silk formation

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Spider silk fibers are produced from soluble proteins (spidroins) in a poorly understood process. They are highly repetitive in sequence, capped by non-repetitive *N*- and *C*-terminal domains (NT and CT). We found that the pH gradient in the silk gland is much broader than previously known. When the pH is lowered a series of protonation events results in dimerization and stabilization of NT. Pre-alignment of NT into weakly associated dimers may prevent premature aggregation and circumvents the need for high diffusion and association rates during the rapid polymerization of spidroins into fibers.[1] CT shows an opposite behaviour in response to lowered pH, it is destabilized and unfolds into thioflavin T-positive β-sheet amyloid-like fibrils, which can trigger silk formation. Carbonic anhydrase activity emerges in the same region of the gland as the effects on NT and CT occur.[2] These events suggest a novel CO_2 and proton dependent lock-and-trigger mechanism of spider silk formation.

[1] N. Kronqvist et al. *Nat Commun* **2014**, *5*, 3254.
[2] M. Andersson et al. *PLoS Biol.* **2014** *(in press)*

Characterization and crystal structure of a fungal glycoside hydrolase family 3 β-glucosidase, Cel3A from *H. jecorina*

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β-glucosidases hydrolyze a β-linkage between two adjacent glucose molecules. The most abundant β-glucosidase in the mesophilic fungus *Hypocrea jecorina* is Cel3A (HjCel3A). We show that increased levels of HjCel3A in a cellulase mixture produced by *H. jecorina* improve saccharification of lignocellulosic biomass for the production of biofuels. In addition, we present structures of HjCel3A from enzymes produced either in *H. jecorina* or *Pichia pastoris* (pp-HjCel3A), with and without glucose complexed in the active site. The HjCel3A structure has a three-domain architecture, as previously observed for two other glycoside hydrolase family 3 β-glucosidases. Biochemical characterization of HjCel3A shows that the enzyme is efficient for hydrolysis of (1,4)- as well as (1,2)-, (1,3)-, and (1,6)-β-D-linked disaccharides. Both HjCel3A structures have *N*-linked glycosylation at *Asn*208 and *Asn*310.

BNB - Oral 3

Magnetic metal oxide based adsorbent for extraction and separation of rare earth elements

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Mesoporous transition metal oxides with high surface area (over 200 m^2/g) can efficiently be produced by a thermohydrolysis approach from solid metal alkoxides precursors.[1] These materials can be made magnetic via insertion of iron oxide nanoparticles. Protection of materials against acid leaching is achieved by deposition of a thin layer of TiO_2. The produced materials are easily modified by grafting of phosphonate ligands leading to creation of hybrid adsorbents conserving the morphology and surface characteristics of the applied oxide matrices. Aminopropyl phosphonic and imino(dimethylphosphonic) acids were used to achieve a proof-of-concept. The obtained adsorbents revealed good adsorption capacity towards the cations of rare earth elements (REE); 0.18, 0.21, 0.23, and 0.24 mmol/g for yttrium(III), neodymium(III), lanthanum(III) and dysprosium(III), respectively. These materials can be used for water purification and for recycling of REE.

[1] G. A. Seisenbaeva et al., *Chem. - Eur. J.* **2014** *(accepted for publication)*

Acceleration of fiber formation for efficient synthesis of functional yeast prion protein nanofibers

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Fiber formation of the yeast prion proteins Sup35 and Ure2 is phenotypically expressed in yeast as the inheritable factors [PSI+] and [Ure3], respectively. Nanofibers are formed by the N-terminal domains of Sup35 (1-61) and Ure2 (1-81), which self-assemble with β-sheet secondary structure. Biotechnological utilization of these nanofibers requires simple means to regulate their synthesis. We studied the induction of fiber formation through sonication, agitation, seeding, changes in pH or the addition of the detergent SDS. A direct comparison of Sup35 (1-61) and Ure2 (1-81) reveals that Sup35 is the better candidate for biotechnological applications if controllability and fibrillation speed are the decisive factors. Co-fibrillation of Sup35 (1-61) with Sup35 (1-61)-Z-domain dimer resulted in doped nanofibers in less than two hours that are fully functional IgG binders. Sup35 fibers can furthermore be exploited as stable physical linkers between two functional entities. Equipped with Q-dots and magnetic beads through a biotin-streptavidin bond, Sup35 fibers offered a linkage that did not deteriorate for several months. With the ability to rapidly assemble functional nanofibers, we provide a basic concept for countless possible biotechnological applications.

BNB - Oral 4

Sustainable biodiesel and animal feed from lignocellulose with oleaginous yeasts

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Technologies based on non-food, lignocellulose biomass are especially promising for reaching a sustainable economy. Methods to convert the cellulose to valuable compounds such as ethanol have been established. However, the hemicellulose and lignin fractions are still underutilised. We present research on converting hemicellulose sugars to lipids for biofuel and animal feed (mainly fish feed) production. Oleaginous yeasts can upon nitrogen limitation convert carbohydrates into fatty acids at the highest known specific rates and the fatty acid content can exceed half of the total biomass of the cell. Lignocellulose is usually poor in nitrogen and, therefore, appropriate to be converted to lipids. On the other hand it contains inhibitors that might disturb yeast growth and lipid production. We are using the hemicellulose fraction of pre-treated lignocellulose to produce fatty acids, including investigating regulation of yeast physiology which determines the amount of lipids produced and the saturation degree of fatty acids. Omega-3 fatty acids are of special interest for the production of animal feed. First results indicate that it is possible to manipulate the yeast metabolism to generate longer chain omega-3-fatty acids.

Novel strategies to reduce diffuse emissions of micropollutants from on-site sewage treatment facilities

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In Sweden, approx. 700 000 households (~10%) are not connected to public sewage treatment plants (STPs). Conventional centralised STPs are not economically feasible for sanitation of these sparsely populated areas, and therefore more cost-effective small-scale treatment facilities are used. Most of these consist of a sludge separation with subsequent treatment with sand beds, where the treated waste water thereafter is drained to surface water. The Formas project RedMic will identify emissions of organic pollutants from OSSFs by using target and non-target screening mass spectrometry (MS) methodologies and will study the fate of these micropollutants (MPs) in the environment. For this purpose, *in silico* tools will be combined with field and experimental studies to evaluate the impact of emissions from OSSFs on the receiving aquatic environment.

The ecotoxicological interplay between nanoparticles and further environmental parameters

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Nanoparticles are used in a broad range of products, which ultimately enhances the likelihood for nanoparticle-release into freshwater ecosystems requiring a characterization of the environmental risks associated with their use. However, environmental parameters (ENPs) may influence their fate and finally their ecotoxicological potential. Natural organic matter, for instance, covers the ENPs' surface stabilizing particle size due to steric or electrostatic repulsion, which may reduce the ecotoxicity of nanoparticles. In contrast, sunlight (i.e. ultraviolet light) may activate the photocatalytic properties of nanoparticles, which finally lead to the formation of reactive oxygen species (ROS). Although, society is taking advantage of this process during decontamination, ROS can directly harm aquatic life. In addition, nanoparticles may affect the bioavailability of other chemical stressors such as heavy metals or organic contaminants. These aspects will be discussed involving recent experimental evidences.

Session 3

Imaging, Analyses, Function

"Maybe we should run a level 3 diagnostic on all key systems?"

Lt. Cmdr. William T. Riker
Cause and Effect, Star Trek: the Next Generation

Spectrally and time-resolved fluorescence imaging in molecular diagnostics

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New classes of fluorescent probes for bio-sensing are continuously being developed, along with new optical microscopy modes of measurement. It is of interest to combine time- and spectrally resolved imaging, as both can be obtained from fluorescence, and even from the very same laser scanning microscope and sample. Specifically, it will be presented novel spectral image analysis tools based on spectral correlation. The latter analysis technique allows us to quantify spectral content and also discern very weak signals from a noisy background, such in the case of *e.g.* in vivo based measurements.

It will be given a brief introduction to fluorescence life-time imaging (FLIM) and shown how this in combination with hyperspectral imaging analysis can give additional information on molecular and dynamic processes. Some recent examples are given from systems investigated with multifunctional imaging probes, such as paramagnetic free spin-labels, clusters or nanoparticles, in combination with fluorescence. Here it is possible to map the microscopic chemical spectroscopic properties obtained by the optical techniques, by employing macroscopic 3D localization using magnetic resonance methods. Examples are taken from the FP7-LUPAS project,[1] aimed at developing new fluorescence molecular tools for diagnostics of amyloid protein states in mouse models of Alzheimer disease, and a project aimed at the visualisation of oxidative stress in human *ex vivo* biopsies of atherosclerotic plaques.

[1] www.lupas-amyloid.eu

Alcohol oxidase – a possible extracellular source H_2O_2 during decay of wood by the brown rot fungus *G. trabeum*

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Brown rot fungi are the principle cause of the highly destructive form of decay observed in wooden constructions where they oxidatively degrade wood cell components causing rapid loss of wood strength. The molecular mechanisms and enzymatic systems that these fungi use for rapid and selective depolymerization of wood cellulose during decay have been highly debated and controversial and are still not fully understood. In most models, a central role for a low molecular weight, immediate depolymerising agent that can easily penetrate wood cell walls is given to hydroxyl radicals generated from extracellular H_2O_2:

$$H_2O_2 + Fe^{2+} + H^+ \rightarrow \cdot OH + Fe^{3+} + H_2O \text{ (the Fenton reaction)}$$

Key to all processes is however a source of H_2O_2 and regeneration of Fe^{2+} and a number of non-enzymatic systems have been implicated including extracellular phenolate biochelators, extracellular Fe^{3+} chelating/reducing glycopeptides and peptides. In contrast with non-enzymatic processes we have looked for possible enzymatic sources of H_2O_2 in *Gloeophyllym trabeum*, one of the most frequently reported brown rot fungi causing decay in houses.

Atomic force microscopy: innovations in life science and polymer research

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Atomic force microscopy (AFM) has long been recognized as a useful tool for visualizing various samples with a nanometer resolution. Recent developments at Bruker including introduction of the proprietary PeakForce Tapping® technology made possible easy high resolution imaging and simultaneous quantitative nanomechanical mapping of material properties, including modulus and adhesion.

In our presentation we will introduce how the latest PeakForce Tapping® technology could be utilized in characterizing polymers and various biological samples ranging from single molecules up to living cells.

IAF - Oral 3

Functional analysis of glycosaminoglycan sulfatases from *B. thetaiotaomicron*

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It was recently reported that sulfatases play a key role in the adaptation of a major human commensal bacterium, *Bacteroides thetaiotaomicron*, to its host.[1] Sulfatases catalyse hydrolysis of sulfate groups from a broad range of substrate molecules including large macromolecules such as mucins or glycosaminoglycans (GAGs). We present the identification and biochemical characterization of four novel GAG specific sulfatases from *B. thetaiotaomicron*. Two of them are 6-*O*-sulfatases with a strict specificity for either gluco- or galactosaminoglycans. The third, identified as a Δ-4-hexuronate-2-*O*-sulfatase, remove sulfates from a hexuronate unit independent of the parent GAG. Whereas these three enzymes possess strictly exolytic activity, like all bacterial sulfatases reported so far, an endosulfatase was also identified, which removes sulfate groups in the 4-*O*-position of *N*-acetylgalactosamine and is the first bacterial GAG endosulfatase reported to date active at polymer level.

[1] B. Benjdia et al. *J. Biol. Chem.* **2011**, *286*, 25973-25982.

SafeDrink: Integrated chemical and toxicological methods for early detection of hazardous chemicals in drinking water

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Recently several water sources had to be shut down because of pollution of perfluoroalkyl substances (PFASs). The occurrence of the pollutants was found by chance, and the drinking water treatment plants were not aware of the risks. The main objective of *SafeDrink* is to develop methods for assessment of hazardous chemicals in drinking water by integrating chemical analysis and in vitro toxicity tests. We present the overall methodology of *SafeDrink* and the first results from two of its sub-projects. Method development for pre-concentration of pollutants in the field using passive samplers is demonstrated to be preferred over conventional grab sampling. Similarly, in a water purification study, a combination of alternative methods improved the treatment efficiency of removing organic micropollutants including PFASs.

IAF - Oral 4

Drinking water for Stockholm from Lake Mälaren even in the future

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For drinking water producers elevated concentrations natural organic matter (NOM) in potable water a concern. NOM can cause discoloration of the water and the smell and taste disorders, and act as substrates for microbial growth in the pipeline. Disinfection with chlorine causes formation of trihalomethane, which in some cases are suspected to give rise to carcinogenic substances in drinking water and other byproducts.[1] Lake Mälaren is the most important aquifer for the entire Mälardalen. Unlike other surface waters used for drinking water Lake Mälaren has a very long residence where the formation of autochthonous carbon can be significant during the summer and autumn.[2] Here we evaluate the performance of a hollow fiber membrane pilot scale filter for lake water organic matter removal and characterize organic matter from Mälaren.

[1] E. Lavonen et al. *Environ. Sci. Technol.* **2013**, *47*, 2264-2271.
[2] S.J. Köhler et al. *PLOS ONE* **2014**, *8*, e70598.

Development of antibodies for determination of alkylresorcinol metabolites in urine and elucidation of ELISA cross reactivity

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Alkylresorcinols (ARs) are amphiphilic phenolic lipids and their two main metabolites, 3-(3,5-dihydroxyphenyl)-propanoic acid (DHPPA) and 3,5-dihydroxybenzoic acid (DHBA) may be used as biomarkers of whole grain wheat and rye intake. AR metabolites levels are currently measured by chromatographic techniques, but for samples from large epidemiological studies, immunoassay techniques are warrented. The aim of this work was to develop antibodies against DHBA and DHPPA to be used for ELISA analysis. Good calibration curves were obtained for ELISA using alkaline phosphatase (AP) conjugates. These compounds showed high cross-reactivity in ELISA and may explain the several-fold higher results obtained by ELISA compared with GC-MS.

[1] M. Franek et al. *Anal. Chem.* **2006**, *78*, 1559-1567.
[2] A. Koskela et al. *Clin. Chem*. **2007**, *53*, 1380-1383.
[3] R. Landberg et al. *Am. J. Clin. Nutr.* **2008**, *87*, 832-838.
[4] M. Marklund et al. *J. Chromatogr. B* **2010**, *878*, 888-894.

Session 4

Food, Feed, Natural products

"Quadrotriticale is a high-yield grain, a four-lobed hybrid of wheat and rye. A perennial, also, I believe."

Lt. Cmdr. Spock
The Trouble with Tribbles, Star Trek

Food structures and properties

Maud Langton
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Food biophysics, the relationship between food microstructure and the functionality in complex food matrices, will be explained and exemplified by showing the impact of macro- and microstructure on rheology, sensory, and other functional properties in various food applications such as dairy, cereals, starch, fruits, vegetables, and emulsions. More fundamental research on biopolymer systems at different length scales is needed in order to create a base for understanding phenomena occurring in complex food systems. The microstructural competence, as well as cereal knowledge, is needed to understand the breakdown of food during digestion. By using immunolabelling, the spatial distribution of targeted compounds (*e.g.* arabinoxylan and β-glucans) can be visualized. Currently work is been done to develop and characterize stomach viscosity-enhancers to delay gastric emptying as a means of enhancing satiety, building on previous work and introducing new concepts of gastric structuring.

Chemical side of starch-based films and coatings with improved barrier properties

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Starch is a promising biopolymer for the production of eco-friendly materials. It is cheap and forms strong films with excellent oxygen barrier properties, a desirable trait for food packaging. However, the hydrophilicity of the biopolymer renders the materials moisture sensitive. In our research we have studied the impact of cross-linking starch with citric acid and acetylation on chemical structure in starch-based solution-cast films and coatings.[1-4] The simultaneous cross-linking reaction and hydrolysis of starch by citric acid could be controlled by temperature and pH, and the process could thereby be adjusted to suit industrial conditions. Cross-linking occurred at temperatures as low as 70 °C and hydrolysis could be kept at a minimum at pH 4. In addition, analyses of barrier properties showed that cross-linking had a positive effect on water vapour transmission rate. The two processing techniques studied had different effects on both chemical and barrier properties. In addition, the botanical origin of starch was found to influence barrier properties.

[1] C. Menzel et al. *Carbohydr. Polym.* **2013**, *96*, 270-276.
[2] E. Olsson et al. *Carbohydr. Polym.* **2013**, *98*, 1505-1513.
[3] K. Koch et al. J. *Renew. Mater.* **2014**, *2*, 34-144.
[4] C. Menzel & K. Koch *J. Appl. Polym. Sc. (accepted for publication)*

Responses to different dietary sources of essential nutrients in salmonids

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The aim of the studies is to elucidate the effect of different protein and lipid sources on the liver and muscle metabolic profile of salmonids, specifically Arctic char. To address these issues, fish are fed different diets e.g. including linseed- and rapeseed oil as lipid combined with fish and krill oil and krill, mussel and fish meal as protein source during fifteen weeks to one year. Also, microbial sources of minor compounds (e.g. astaxanthin, beta carotene), lipids and proteins can be evaluated. At the end of the feeding trials, lipids and amino acids as well as aqueous and chloroform extracts are analysed. The use of ^{1}H NMR technology in fish studies has shown a high potential for compositional analysis of muscle, plasma and liver. Liver is a key organ in connection with biosynthesis and metabolism; it shows the highest metabolic rate in the fish and was therefore chosen as a metabolic target for analysis. Analysis of the white muscle tissue provides the metabolic response to the diets, as well as describes the flesh quality for human consumption.

FFN - Oral 3

Mass spectrometry strategies for metabolite identification in metabolomics analysis

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Metabolomics, the quantitative analysis of all the endogenous metabolites in a biological system, provides biochemical information that can be linked to particular phenotypes. These links can be used to identify biomarkers or connected to gene-, protein- or other meta-data in explorations of targeted biological processes. One of the most challenging aspects of metabolomics is characterizing the huge numbers of metabolites in biological samples. Here, we will present different mass spectrometry based strategies for characterizing metabolite composition in various biological samples. The strategies involve both combined GC-MS and LC-MS. The LC-MS includes exact mass determination and tandem mass spectrometry, together with mass spectra interpretation and compound data base searches. Furthermore, a novel software strategy for processing GC-MS data will be presented, resulting improved amount and quality of information that can be obtained from GC-MS based metabolomics analysis.

Cholesterol is a metabolic precursor to the toxic glycoalkaloids in potato

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Steroidal glycoalkaloids (SGA) are toxic secondary metabolites naturally occurring in the potato, as well as in certain other *Solanaceous* plant species, including tomato, eggplant and pepper. To investigate the steroidal origin of SGA biosynthesis, cut potato shoots were fed cholesterol labelled with deuterium (^{2}H) in the sterol ring structure, or in the side chain, and analysed by GC-MS and LC-MS/MS. When feeding ^{2}H-labelled cholesterol solubilised in Tween-80, minor amounts of ^{2}H-labelled SGA (α-solanine and α-chaconine) were identified in cholesterol-treated shoots, but not in blank controls. Solubilising the labelled cholesterol in methyl-β-cyclodextrin instead of Tween-80 increased the levels of labelled SGA up to 100-fold, and about 1 mole% of the labelled cholesterol was recovered as labelled SGA in potato leaves.[1]

[1] E. Petersson et al. *PLOS ONE* **2013**, *8*, e82955.

FFN - Oral 4

Massive deciphering of yeast volatiles attractive to pest insects

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For decades, the interactions between insects and microorganisms have been known, but in the area of plant protection, sadly overlooked. In recent time, the "-omics" methods and tools have made it possible to decode these interactions. Mutualistic yeast and yeast-like fungi are food sources and act as oviposition cues, possibly even to the extent of being the main contributor to the unique flavours and scents of the insects' host plants. One practical application of these insights is a recently published method combining mutualistic yeast and insect pathogenic virus.[1] Larval feeding and attraction assays show differences between closely related yeast species. Yeast volatile profiles are highly complex, but out of the hundreds of components emanating from the yeasts, only a fraction are believed to cause these differences in behaviour. Finding these key compounds is problematic, as abundance does not imply importance, and established laboratory techniques used with adult insects are inapplicable to larvae. By using automated deconvolution and integration of GC/MS data from nine yeast species it became possible to qualitatively compare the "complete" volatile metabolomes of the yeasts without the need to first identify every component.

[1] A. Knight & P. Witzgall. *J. Chem Ecol.* **2013**, *39*, 1019-1026.

Catch and release – how to efficiently trap, analyze and formulate plant odors

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Volatile collection for chemical analysis of plant odor can be done in various ways. The volatiles can be collected *in situ*, i.e. in the field, or the plants can be brought to the lab. The plant material is enclosed in "odorless" cooking bags, in order to minimize background contaminants. Charcoal filtered air is introduced at the bottom of the bag, passes over the plant and brings the released volatiles across the bag to the adsorbent column. The adsorbet is packed in polytetrafluoroethylene tubes and connected to small vacuum pumps. The volume of the cooking bag is minimized, and the air flow through the column is around ten per cent of the enclosure volume per minute, to reduce the risk for break-through of the most volatile compounds during the aeration.

After elution of volatiles, and eventually concentration, the qualitative *and* quantitative analyses are made by combined GC-MS. Not only the identification, but also the proportions of the collected volatiles are often necessary for optimal bioassay of a formulation. The method we have successfully used for decades are cotton lined polytetrafluoroethylene tubes: "wick-baits". The compounds to be tested are dissolved and homogenized in an alkane depending on for how long the bait is supposed to last.

Poster session

Including all session topics

"There's coffee in that nebula."

Capt. Kathryn Janeway
The Cloud, Star Trek: Voyager

Poster SES-01

Calibration and field evaluation of passive samplers for monitoring pesticides in water

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Passive sampling is a promising tool for monitoring of pesticides in water with minimal infrastructure and detection of contaminants at low, environmentally relevant concentrations. Passive sampling is based on an in-situ deployment of devices/sorbent capable of accumulating contaminants freely dissolved in water. Such accumulation occurs via diffusion, typically over periods of days to weeks, and can be described by the compound specific sampling rate, which is the equivalent volume of water accumulated by the sampler per unit of time. In this study, passive samplers were characterized for over 100 individual pesticides in the water phase. In addition, passive samplers were applied in two Swedish river systems and the concentration was compared to active sampling. Sampling rates and polymer-water partitioning coefficients for five different passive sampler types will be presented. Overall, the results of this study will improve our understanding of the concept, challenges and application of passive sampling for future monitoring strategies of a broad range of pesticides in water.

Microbial energetics of soils exposed to different temperatures and land uses

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Soil organic matter is the largest carbon pool in terrestrial ecosystems, being 2-3 times the amount of carbon in the atmosphere. The fate of soil organic carbon in an ecosystem is determined during its decomposition by microbial metabolic activity. Temperature changes may alter both microbial metabolism as well as community composition of active microorganisms. Energy is required to maintain metabolism, and to understand soil microbial energetics and its temperature dependence may improve our knowledge of the global carbon cycle and help in refining climate change modelling.

We investigated microbial energetic patterns of soils exposed to temperatures (5-20 °C) under different land uses by isothermal calorimetry. Soil samples were taken from forest, arable, grassland and ley farming long-term research sites situated in a boreal climate. We determined the heat signals for those samples after soil amendments with different substrates representing simple to complex organic matter. In addition, respirometric measurements were performed parallel on separate soil samples.

Poster SES-02

Poster SES-03

Amendment effects on arsenic uptake in paddy rice – deciphering the regulating mechanisms

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Rice is the primary food source in South and South-East Asia, an area affected by natural arsenic contamination of soil and water. Mitigating arsenic uptake in rice requires an understanding of the regulating mechanisms in the rhizosphere that are responsible for arsenic migration from soil into rice roots. We approach this challenge through coupling spatially resolved analyses with time series and end-point bulk measurements of arsenic in the solid/aqueous phase in soil and plant.

In a pot trial with arsenic contaminated soil from Cambodia, we tested various amendments and found that charred rice straw decreased the arsenic uptake more than charred rice husks. Preliminary results from XRF mapping and XANES analyses suggest that arsenic adsorption to sulfhydryl groups on the char in combination with sulfide precipitation increased arsenic partitioning to the solid phase in the char treatment. Also, the mobilization of arsenic was delayed in the charred straw treatment, suggesting that the timing of arsenic release relative to plant growth stage could be another contributing factor.

Are Al-hydroxy interlayered clays important for phosphorus sorption in soils?

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Phosphorus is one of the main elements promoting the observed eutrophication and algal blooms observed almost every year in the Baltic Sea. The major part of the phosphorus transported to the sea originates from arable lands, where clay soils have been identified as high risk areas. The processes responsible for phosphorus retention in agricultural soils are not completely understood. The aim with this abstract is to *i)* present mineralogy in soils and the clay fraction from six soils included in a long-term fertility experiment, *ii)* evaluate how phosphorus added by fertilization have been bound in these soils, and *iii)* present some preliminary results indicating the importance of hydroxy interlayered clay minerals in soil for phosphorus sorption. The phosphorus speciation, as determined by XANES spectroscopy, showed that the phosphorus added by long term fertilization mainly was adsorbed to aluminium (hydr)oxides, but also precipitated as iron and calcium phosphates.

Poster SES-04

Poster SES-05

Carbon availability and nitrogen source affects chemical composition of ectomycorrhizal fungi in pure culture

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FTIR spectroscopy is a commonly used technique capable of distinguishing the principal chemical classes in cell walls, through the characteristics of their structural chemical bonds. For fungal species forming symbiosis with plant roots, the so called mycorrhizal fungi, this technique had not been commonly used. Ectomycorrhizal (ECM) fungi, dominating in the boreal forest ecosystem, contributes significantly to carbon fluxes[1] and build-up of soil organic carbon.[2]

Our aim was to determine if FTIR spectroscopy of ECM fungi grown in pure culture could be used to *i)* distinguish between different ECM fungal species when grown under the same conditions, *ii)* find differences in cell wall composition related to carbon availability, nitrogen source, temperature and time, and *iii)* relate the potential species-specific differences in chemical composition due to carbon availability to turnover of fungal mycelium. Preliminary results will be discussed.

[1] Bhupinderpal-Singh et al. *Plant Cell Environ.* **2003**, *26*, 1287-1296.
[2] K.E. Clemmensen et al. *Science* **2013**, *339*, 1615-1618.

Crystallization and a preliminary crystallographic analysis of manganese-lipoxygenase

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Oxygenation of polyunsaturated fatty acids results in plants and animals to biologically significant mediators, *e.g.* prostaglandins, leukotrienes, jasmonic acid, and jasmonic acid hydroperoxides. These mediators are precursors of signal molecules in animals, plants, and fungi and may take part in inflammation and the chemical warfare between plants, fungi, and other microorganisms. Lipoxygenases constitute a family of non-heme metal enzymes with catalytic iron or, occasionally, catalytic manganese lipoxygenases (LOX). The 3D structures are available of at least nine lipoxygenases from plants and animals, but 3D structures of fungal lipoxygenases have not yet been reported. LOXs consist of two domains, a domain with β-barrel and a catalytic domain with α-helices and a metal center. The iron is coordinated to three *His* residues, the carboxyl oxygen of the C-terminal amino acid, and usually to a distant *Asn* residue. To understand the structure-function differences between the manganese and iron LOXs, we have made an attempt to crystallize the manganese-LOX of *Gaeumannomyces graminis* for structure determination.

Poster SES-06

Organic matter removal for drinking water production

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The amount of dissolved organic carbon (DOC) has risen in our lakes during the past 20 years and it has also changed in character. DOC causes problems for water treatment plants that are using surface water as a drinking water source. It gives the water odour, taste, colour, leads to a higher need of precipitation chemicals, more sludging, and greater formation of potentially harmful disinfection products. With the changes in both amount and character, current water treatment techniques need to be improved.

In this study, two conventional water treatment techniques (precipitation with iron chloride and precipitation with aluminium sulfate) and two more modern techniques (ion exchange with MIEX® and membrane filtration) were examined. Six waters with extreme types of DOC were used, including algogenic water, wastewater, and water from mire, in order to have a wide range of SUVA-values. SUVA is the ratio between absorbance at 254 nm and the content of DOC. SUVA gives an indication about the distribution of allochthonous and autochthonous matter. Waters with SUVA values >3 were more easily treated than water with lower values, but the relation was not linear. There was a correlation between absorbance and the amount of DOC, which makes it possible to do online reading of absorbance and translate the values into amount of DOC.

Per- and polyfluoroalkyl substances (PFASs) in Swedish rivers and the Baltic Sea

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Per- and polyfluoroalkyl substances (PFASs) are ubiquitously distributed in the environment, and are of concern due to their persistence and bioaccumulative and toxic properties.[1-3] The aim of this study was to investigate the occurrence of PFASs in Swedish rivers and the Baltic Sea. Water samples were collected at 44 river sites along the Swedish coast, primarily at river mouths, and at 18 sampling sites in the Baltic Sea between September and October 2013. The samples were filtered through glass fiber filters and extracted using solid phase extraction. The analyses of PFASs were performed using high performance liquid chromatography coupled mass spectrometry (HPLC-MS/MS). Preliminary results show that the levels of PFASs vary depending on the water flow and anthropogenic impact.

[1] J.W. Martin et al. *Environ. Toxicol. Chem.* **2003**, *22*, 196-204.
[2] L. Ahrens et al. *J. Environ. Monitor.* **2011**, *13*, 20-31.
[3] J.P. Giesy et al. *Rev. Environ. Contam. Toxicol.* **2010**, *202*, 1–52.

Poster SES-09

Phosphate effects on cadmium sorption to ferrihydrite

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Elevated cadmium concentrations in soil is a problem both in soils contaminated by industrial activities and in agricultural soils. Cadmium(II) ions adsorbs to iron oxides in soil and this sorption may be affected by the soil phosphorus content. To elucidate the effects of phosphate on cadmium sorption to iron oxides a combination of batch experiments, EXAFS measurements, and surface complexation modeling with the CD-MUSIC model was performed. Sorption experiments with cadmium(II) ions and ferrihydrite, with and without addition of phosphate, covered a pH range of about 4 to 7. Sorption of cadmium to ferrihydrite was enhanced by phosphate at about pH <7. The sorption of cadmium in single sorbate systems was attributed to bidentate cadmium/ferrihydrite surface complexes. A surface complexation model with a bidentate cadmium/ferrihydrite complex provided a good model fit for the single sorbate systems. However, the EXAFS results showed a change in cadmium(II) coordination when phosphate was present. This could be explained by the introduction of a ternary surface complex in the surface complexation model. In conclusion, geochemical models simulating trace element behavior in environments rich in iron and phosphorus need to account for ternary metal-phosphate surface complexes to properly describe partitioning of metals between solution and solid phase.

Poster BNB-01

Investigation of the microbial storage flora of birch and spruce sawdust

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Sawdust is a rest product from forest industry that holds a great potential for industrial application both as raw material for building and furniture production, for heating and electricity production and for biofuel production. Before utilising sawdust for the different purposes the material has to be stored for varying time periods. During those periods, occasions of microbial infections have been reported by the production personnel, e.g. moulding or occurrence of bad smells.

Up to now, no investigations of the microbial storage flora on sawdust have been performed. We investigated the microfungi and bacterial population on birch and spruce sawdust stored for twelve weeks at 2, 20, and 37 °C. Rather high numbers of bacteria were found in the storage systems that were higher than those of moulds and yeasts. Yeasts were only found in sawdust stored at 2 °C. Many of them were cryophilic and have earlier been associated with insects living on wood. At higher temperatures, moulds of the genera *Penicillium* and *Aspergillus* were dominating. The impact of the microflora on the stored sawdust on its further application will be discussed.

Synthesis and characterization of the composites based on cotton fibers and nanocrystalline titania

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During the past decade titania-based coatings with high specific surface area and narrow pore size distribution have provided many new prospects for practical applications. We report a novel method of obtaining TiO_2 modified cotton fibers possessing high photocatalytic activity and antibacterial properties. To obtain titania particles a low-temperature sol-gel synthesis was used, leading to an anatase/brookite modification in solution. Further treatment of cellulose fibers by nanocrystalline titania hydrosol using a cross-linking agent yielded nanoparticles on the surface of the cotton fiber. The physical and chemical properties of hybrid nanomaterials were investigated by FT-IR, thermogravimetric analysis, low-temperature adsorption/desorption of nitrogen, atomic-force and scanning electron microscopy. The FTIR spectroscopy revealed that upon adding BTCA as a cross-linking agent to TiO_2 hydrosol, an absorption band is observed indicating the formation of Ti-O-C interactions. The modified TiO_2 fibers have bacteriostatic effect, inhibiting the growth and development of pathogenic bacteria in the fight against hospital infections.[1]

[1] O.L. Galkina et al. *Surf. Coat. Technol* **2014**, *253*, 171–179.

Poster BNB-02

Poster BNB-03

Crystal structure of a glycoside hydrolase family 3 β-glucosidase from the thermophilic fungus *R. emersonii*

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A glycoside hydrolase (GH) family 3 β-glucosidase from the moderately thermophilic fungus *Rasamsonia emersonii*, *Te*Cel3A, was heterologously expressed in *Hypocrea jecorina*. The expressed protein was purified, crystallized and the structure of the enzyme was solved by X-ray crystallography to 2.2 Å resolution. The structure was solved by molecular replacement. This is, to our knowledge, the first structure of a three-domain GH family 3 β-glucosidase that contains a novel feature in the form of a very extended loop insertion in the middle of the third, *C*-terminal domain. This loop folds back on top of and follows the surface of the *N*-terminal domain, which contains the substrate-binding pocket of the enzyme. A second ligand bound structure of the enzyme with β-D-glucose bound in the active site of the enzyme, was also solved to 2.6 Å resolution. There are a total four non-crystallographic symmetry related (NCS) molecules in the *Re*Cel3A crystal structure. These four NCS molecules form two apparent dimers in the structure. This finding is in consistence with previously published result that *Re*Cel3a often appear as a dimer in solution.

New structural insights into GH6 cellobiohydrolases

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Cellulases, glycoside hydrolases that catalyze the degradation of cellulose, are classified as either endoglucanases or cellobiohydrolases (CBHs) based on their architecture and mode of action on the cellulose. CBHs are typically major components of natural enzyme cocktails for biomass degradation. Their active sites are enclosed in a tunnel, enabling processive hydrolysis of cellulose chains. Glycoside hydrolase Family 6 (GH6) CBHs act from non-reducing ends on the cellulose chains and utilize an inverting mechanism to cleave the β-1-4 linkage. GH6 CBHs are present in many cellulolytic fungi and bacteria. The bacterial *Thermobifida fusca* Cel6B (TfuCel6B) exhibits a longer and more enclosed active site tunnel than its fungal counterparts e.g. Cel6A/CBH2 from the ascomycete *Hypocrea jecorina*. The structures of the wild-type and catalytically deficient supports the presence of a Grotthuss proton transfer chain for a nucleophilic attack on the anomeric carbon. The observed sugar binding together with crystallographic waters in one of the structrues enabled the construction of a model of the α-anomer product after hydrolysis. With simulation, we demonstrate that both loops can readily open to allow product release with equal probability in solution or when the enzyme is engaged on cellulose.

Poster BNB-04

Poster BNB-05

Polyoxotitanate nanoclusters from reaction of titanium(IV)ethoxide and amino phosphonate ligand

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Nanotechnology is a big and important research field, in part dedicated to find and determine new structures of nanoclusters. Polyoxotitante nanoclusters are interesting thanks to their interaction with biomolecules and also for their potential use as a part of anodes in photovoltaic cells. In this work, crystals of polyoxotitanate nanoclusters were obtained in room temperature using reaction of titanium(IV)ethoxide, $Ti(OEt)_4$, with amino phosponate ligands. The crystal structure was determined as novel using SHELXTL. Potential areas of application of the new material is currently being studied.

Magnetic enzyme formulations for environmental and biomedical use

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Magnetically retrievable formulations of urease perspective for biomedical and environmental use were constructed by enzyme immobilization on the surface of magnetite nanoparticles functionalized by siloxane layers with active thiol or thiol-and-alkyl moieties. Immobilization of urease was carried out in different ways for comparison: by adsorption, by entrapment during the hydrolytic polycondensation reaction, or by covalent bonding. Entrapment bound high amounts of enzyme (more than 700 mg per g of carrier), but its activity was decreased compared to the native form to between 18 and 10%. In case of covalent binding of urease using Ellman's Reagent, the binding of enzyme was almost as efficient as in case of entrapment but its residual activity was 75%. The residual activity of urease immobilized by adsorption on the surface of thiol-functionalized particles was truly high as compared to native enzyme (97%), but binding was significantly less efficient (46%). Introduction of alkyl functions permitted to increase the amounts of adsorbed enzyme but its activity was somewhat decreased.[1]

[1] R. Pogorilyi et al. *J. Mater. Chem. B* **2014**, *2*, 2694-2702.

Poster BNB-06

Poster BNB-07

Nanostructured matrices for bacterial encapsulation

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One of the greatest barriers to successful use of biocontrol agents for in field applications is the lack of reliable methods and procedures that consistently give the desired activity and efficiency. The EU ERA_NET program BAC-COAT aims to develop principle new formulations where biocontrol bacteria are encapsulated in inorganic and/or organic matrices to achieve long-term storage stability and functionality in the field. The encapsulation concept focuses on biocompatible mineral nanoparticles and polyelectrolyte multilayers that form a protecting shell around the microorganism, with good mechanically stability, selective permeability and material properties that enable controlled release of the bacteria cells as a response to an external stimulus. Well characterised biocontrol bacteria, representing different phylogenetic and morphological groups including Burkholderia phytofirmans and *Paenibacillus* sp., are used as model organisms to understand the mechanisms of the bacteria-capsule interface and to identify approaches to optimize storage stability and efficiency at its application. The BAC-COAT program is a collaboration between research institutes and the industry and involves both fundamental and applied research.

Nanotitania-aided colonization of *B. napus* by growth-promoting rhizobacteria *B. amyloliquefaciens* strain UMBC5113

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The surface activity of particles and molecules of this size is greatly enhanced compared to bulk. Increased surface-to-volume ratio gives atoms at the surface less neighbor interference and lower coordination, resulting in increased affinity to foreign atoms. Quantum size effects occurring in conducting materials where electrons move freely also contribute to increased surface reactivity.[1] Our titania nanoparticles, with positive surface charge, adhered bacteria of spatially variable charge to rape seed (*Brassicae napus*) roots which have negative charge. These particles have been described earlier and proven to be biocompatible.[2,3] A SEM study showed increased fixation of clusters on the roots and coupled EDS-analysis confirmed the presence of titanium. By GFP tagging our bacterium we illustrated the effect of increased adherence by our titania nanoparticles. We quantified the amount of bacteria by washing the roots and counting CFUs.

[1] E. Roduner *Chem. Soc. Rev*. **2006**, *35*, 583-592.
[2] G.A. Seisenbaeva et al. *Nanoscale* **2013**, *5*, 3330-3336.
[3] V.G. Kessler et al. *Angew. Chem. Int. Ed.* **2008**, *47*, 8506-8509.

Poster BNB-08

Poster BNB-09

Hybrid nanoadsorbents for extraction/separation of REEs

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Rare earth elements (REEs) have become increasingly important over the last decades due to their wide applications fields such as electronics, biomedicine, catalysis, nanotechnology, engineering, and production of luminescence compounds. These applications make the availability of REEs very important and consequently also their extraction and separation for recycling. In this work, magnetic hybrid nanoadsorbents functionalized with different organosilane derivates were synthesized and their affinity to REE cations in solution were tested. Fe_3O_4 magnetic nanoparticles (NPs) were chosen because of their magnetic properties and stability. These were synthesized and coated with a thin layer of SiO_2 and this silica coating process was optimized, resulting in highly stable core-shell Fe_3O_4@SiO_2 NPs. Three different organic chelates were synthesized and attached to the surface of core-shell stuctures as well as to the surface of SiO_2 NPs, which were used as prototypes for adsorption. Succesful surface ligand grafting was assessed by FTIR, TGA and ^{1}H and ^{29}Si solid state NMR. In dynamic conditions, REE uptake was studied by SEM-EDS analysis whereas for static conditions, complexometric titrations of mother liquors were carried out at different times, observing a quick and high uptake capacity for some of the organic chelates grafted nanoadsorbents.

Ethanol production from a lignocellulose-based substrate by the non-conventional yeast *Dekkera bruxellensis*

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The ability of the non-conventional yeast *Dekkera bruxellensis* to outcompete *Saccharomyces cerevisiae* under glucose-limited continuous fermentation with cell recirculation, high ethanol production yields and ability to assimilate cellobiose makes this yeast a promising candidate for ethanol production from lignocellulose. This study investigated the ability of *D. bruxellensis* to adapt to a lignocellulose hydrolysate and how this affected growth and ethanol production. Adaptation of *D. bruxellensis* to lignocellulose hydrolysate by batch and continuous pre-cultivation for 72 and 194 hours, respectively, was demonstrated. Pre-cultivation in lignocellulose hydrolysate resulted in faster growth and higher ethanol production by adapted *D. bruxellensis* as compared to non-adapted cells. Subsequent cultivation of adapted cells in non-selective rich medium resulted in partial loss of obtained phenotype by adapted cells. It was observed that cell adapted by continuous cultivation had a more stable phenotype than cells adapted in batch cultivation. In this case, only slight reduction of initial growth was observed after cultivation of *D. bruxellensis* cells adapted in continuous system in rich medium. These results show that *D. bruxellensis* has a potential for application in ethanol production from lignocellulose-based substrate.

Poster BNB-10

Poster IAF-01

Structural studies of a feruloyl esterase from *F. oxysporum* employing experimental phasing approaches

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Hemicellulose is a heterogeneous group of branched and linear polysaccharides bound via hydrogen bonds to the cellulose fibrils found in plant cell wall. Its degradation is catalyzed by hemicellulases which are key enzymes in the saccharification process of plant biomass. Feruloyl esterases hydrolyse the ester bond between the hydroxycinnamic acids and sugars present in the hemicellulose side chains facilitating the access of hydrolases to the backbone polymers. They are classified into four types (A-D) according to their amino acid sequence identity and substrate specificity.[1] Here we report our structural studies on a type C feruloyl esterase (*Fo*FaeC) from the filamentous fungus *Fusarium oxysporum* which has no close homologue with known 3D structure. Our ultimate aim is to determine the 3D structure of *Fo*FaeC in the native form and in complex with various oligosaccharide analogues in order to elucidate its mode of action.

[1] E. Topakas et al. *Process Biochem.* **2007**, *42*, 497-509.
[2] M. Moukouli et al. *Appl. Microbiol. Biotechnol.* **2008**, *79*, 245-254.

Structural insights into the inhibition of Cel7A by xylo-oligosaccharides

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The filamentous ascomycete fungus *Hycorea jecorina* (previously known as *Trichoderma reesei*) is the predominant source of cellulase enzymes for industrial use.[1] The major enzymes in the cocktail can be divided into endoglucanases that make endolytic cuts in non-crystalline regions to create cellulose chain ends, cellobiohydrolases (CBH) that act processively from chain ends into crystalline regions, and β-glucosidases that hydrolyse cellodextrins to glucose. CBHI (*Hje*Cel7A) in the most abundant enzyme and is responsible for the majority of hydrolytic potential. CBHs are relatively slow and susceptible to inhibition, which is a challenge for industrial utilization of these enzymes. Xylan derivatives in cellulosic biomass have been recognized as potent inhibitors of CBHs.[2] Here, we report 1.4-1.8 Å resolution crystal structures of catalytic domains of *Hje*Cel7A mutants E212Q (nucleophile) and E217Q (acid/base) in complex with xylotriose, xylotetraose and xylopentaose, and preliminary results of inhibition experiments with xylo-oligosaccharides.

[1] C.C. Geddes et al. *Curr. opin. biotechnol.* **2011**, *22*, 312-319.
[2] M.J. Baumann et al. *Biotechnol. biofuels* **2011**, 4, 45.

Poster IAF-02

Molecular recognition by engineered binding proteins

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Engineered binding proteins are in many cases cheap and useful alternatives to physiologically derived antibodies for detection and capture of specific proteins or other molecules. Affibody binders are variants of a small three-helix bundle protein called the Z-domain and they are selected from combinatorial libraries using phage display. The selection of good binding proteins to a given "target" is straightforward. Binding affinities in the low nanomolar range is frequently achieved and the affinity can be improved to the pico- or even femtomolar range using a second library (affinity maturation). We have studied a number of affibody binders engineered for different applications. These include affibody binders to Staphylococcal protein A (biotechnological applications), the human HER2 receptor (cancer diagnostics), and the amyloid-β peptide (Alzheimer therapy). Structural studies reveal the basis for molecular recognition and for how binding affinity was improved by affinity maturation.[1] Our studies have also provided examples of novel and surprising ligand binding modes and how binding affinity can be amplified in repeated multi-domain protein constructs.[2,3]

[1] C. Eigenbrot et al. *Proc. Natl. Acad. Sci. U.S.A.* **2010**, *107*, 15039-15044.
[2] W. Hoyer et al. *Proc. Natl. Acad. Sci. U.S.A.* **2008**, *10*, 1111-1122.
[3] M. Lindborg et al. *J. Prot. Engin. Des. Selct.* **2013**, *26*, 635-644.

The molecular architecture of Aβ protofibrils investigated by solid-state NMR

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The aggregation and fibril formation of the amyloid-β peptide (Aβ) are central in the pathology of Alzheimer's disease and accumulating evidence suggest that the neurodegenerative process is triggered by prefibrillar aggregates, *i.e.* oligomers and protofibrils. We have engineered a variant of Aβ, Aβcc, that allows for preparation of large amounts of protofibrils with properties that are indistinguishabe from those of the wild type peptide.[1,2] We use solid-state NMR spectroscopy to investigate the molecular architecture of Aβcc(1-42) protofibrils. Our results show that the peptide adapts a β-hairpin conformation with high β-strand content in the C-terminal segment. We also detect a significant number of intermolecular contacts involving of the C-terminus of the peptide. Our model provides molecular explanations for several biochemical observations of Aβ aggregation.

[1] A. Sandberg et al. *Proc. Natl. Acad. Sci. U.S.A.* **2010**, *107*, 15595-15600.
[2] A. Dubnovitsky et al. *PLOS ONE* **2013**, *8*, e66101.

Poster IAF-05

Binding of human proteins to neurotoxic Alzheimer amyloid-β protofibrils – identification and binding kinetics

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It is believed that the neurodegeneration of Alzheimer's disease (AD) is linked to the presence of prefibrillar aggregates of the amyloid β-peptide (Aβ) in the brain but the exact role of these aggregates in disease pathology is not fully understood. Any mechanism of AD pathology involving Aβ must proceed via interactions between the Aβ aggregates and other molecules. We used an engineered Aβ variant, Aβ42CC to map the protein interaction network of Aβ protofibrils in human serum and cerebrospinal fluid.[1,2] Many of the 101 proteins that were found to interact with Aβ42CC protofibrils are involved in lipid transport and metabolism, and in hemostasis. Our results also suggest that aggregation of Aβ enhances protein binding, because a smaller amount of proteins bind monomeric Aβ. Taken together, our results suggest that improved understanding of the mechanisms by which Aβ causes cytotoxicity and neurodegeneration might be gained from studies carried out under biologically relevant conditions in which Aβ-binding proteins are present.

[1] A. Sandberg et al. *Proc. Natl. Acad. Sci. U.S.A.* **2010**, *107*, 15595-15600.
[2] A. Dubnovitsky et al. *PLOS ONE*, **2013**, *8*, e66101.

Novel biomarkers of prostate cancer risk: identification using metabolomics approaches

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Prostate cancer (PCa) is the most prevalent cancer form among men in Sweden.[1] Both genetics and environmental factors are associated with an increased risk of PCa.[2] Understanding PCa etiology requires knowledge about gene-environmental interactions at a physiological level, where the metabolic plasma profile can capture these complex interactions.[3] Fasting plasma samples from PCa-cases and their matched controls were recruited from the Northern Sweden Health and Disease Cohort. The samples were collected prospectively, and cases were diagnosed with PCa 5-15 years post sampling while the controls remained healthy. Statistical analysis identified two lysophosphatidylcholines that significantly differed between cases and controls.[4] These findings motivate a more comprehensive investigation of changes in metabolic profile between PCa cases and controls. The same samples are currently analyzed using NMR metabolomics.

[1] The Swedish cancer society **2012** .
[2] R.B. Hayes *Epidemiol. Rev.* **2001**, *23*, 163-167.
[4] J.K. Nicholson et al. *Mol. Syst. Biol.* **2011**, *7*, 525.
[4] J. Storey *J. Roy. Stat. Soc.* **2002**, *64*, 497-498.

Poster IAF-06

Poster IAF-07

Modulation of polycomb repression in *Arabidopsis*

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Polycomb (PcG) complexes mediate epigenetic repression of developmentally regulated genes in higher eukaryotes, governing the onset and maintenance of developmental programmes. Chromatin compaction and gene repression is executed by the polycomb repressive complexes (PRCs) and associated proteins. While the components of PRC2 in plants have been described, knowledge of PRC1 composition remains fragmental.[1,2]. Alteration of developmental programmes is accompanied by chromatin remodelling at PcG targets and PcG repression is likely a major player in modulation of cell fate.[3,4].

We use forward genetic approach and chemical library screening to identify novel modulators of PcG-mediated repression in plants. We screened 10,000 synthetic compounds from the ChemBridge library to identify potential inhibitors of PcG activity in plants. We will present the strategies we used for the identification of the compounds and outlooks for establishing them as chemical modulators of PcG repression in plants.

[1] M. Derkacheva et al. *EMBO J.* **2013**, *32*, 2073-2085.
[2] M. Calonje *Mol. Plant.* **2014**, *7*, 459-471.
[3] C. He et al. *PLoS Genet.* **2012** *8*, e1002911.
[4] E. Apostolou & K. Hochedlinger *Nature* **2013**, *502*, 462-471.

Ligand binding free energy of glycoside hydrolases as a metric for processivity and polysaccharide morphology dependence

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Many glycoside hydrolase (GH) enzymes act via a processive mechanism whereby an individual carbohydrate polymer chain is decrystallized and hydrolyzed along the chain without substrate dissociation. Despite considerable studies, a molecular-level theory of processivity that relates directly to structural features of GH enzymes does not exist. We hypothesize that the degree of processivity is directly linked to the ability of an enzyme to decrystallize a polymer chain from a crystal. We develop a simple mathematical relationship formalizing this hypothesis to quantitatively explain the thermodynamics of processivity.[1] We then calculate the absolute ligand binding free energy of cellulose chains to the biologically and industrially important GH Family 7 processive cellulases with free energy perturbation/replica-exchange molecular dynamics. Taken with previous observations, our results suggest that degree of processivity is directly correlated to the binding free energy of cello-oligosaccharide ligands to GH7s. We conclude that the ligand binding free energy is a key parameter in comparing the activity and function of GHs.

[1] C.M. Payne, et al. *J. Am. Chem. Soc.* **2013**, *135*, 18831-18839.

Poster IAF-08

Poster IAF-09

Volatile organic compounds in exhaled air from dairy cows reflect protein intake and N excretion

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The objective of this study was to evaluate how dietary protein concentration affects the composition of exhaled air in dairy cows. Six mid- to late-lactation dairy cows (Swedish red breed) were offered grass silage at *ad libitum* intake supplemented with different proportions of rolled barley and a commercial protein concentrate. Cows were randomly assigned to one of six sequences in a balanced 3×3 latin-square design with three 4-day periods and three treatments. The treatments were 12, 16, and 20 per cent crude protein in the diet. Measurements and sample collection were made on day 3 and 4 in each period. Samples of exhaled air were collected by face mask in Tedlar bags, transferred to adsorbent tubes and analysed with a gas chromatography–mass spectrometry technique. Urine was collected by spot samples. Results were analysed by the MIXED procedure in SAS. No carryover effects were detected ($P > 0.05$). Milk production averaged 28.5 kg/day and did not differ ($P = 0.36$) among treatments. The results indicate a potential for volatile organic compounds in exhaled air from dairy cows to serve as indicators of dietary protein concentration and nitrogen excretion in the urine.

A pH-responsive polymer sensor for measurements in rumen liquor

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The objective of this study was to evaluate if a wireless sensor based on a mass-changing, pH-responsive polymer and magneto-elastic resonance technique could be used for continuous pH measurements in a rumen *in vitro* environment. Sensors were prepared from foils of magnetic alloy covered by a pH-sensitive polymer. pH detection was based on the fact that thin foils of magneto-elastic materials elongate or shrink upon application of spatially variable external magnetic field. The foil oscillates along its length axis and any material deposited onto the foil will decrease its resonance frequency. Change in pH causes swelling or shrinking of the polymer. A coil positioned to surround the sensor was used to create a magnetic field and detect resonance frequency. Changes in pH, caused by acid inclusion, could be measured adequately in phosphate buffer. In McDougall's buffer, carbon dioxide formation from bicarbonates caused by pH changes disturbed measurements. In rumen liquid pH changes caused by acid and sugar inclusion could be detected but the resonance frequency was not consistently related to pH levels. The described technique seems promising for use in rumen environment but needs further evaluation.

Poster IAF-10

Poster IAF-11

Copper-dependent lytic polysaccharide monooxygenases, what's in it so far?

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Lytic polysaccharide monooxygenase (LPMO) comprise a newly discovered class of enzymes that cleave recalcitrant polysaccharides, *e.g.* cellulose and chitin, by an oxidative mechanism.[1] These enzymes have attracted interest from the biofuel community as they have been shown to act synergistically with conventional cellulases. Very little is currently known about the mechanisms that these enzymes employ, but recent industrial developments indicate that they will be of major importance for the production of biofuels. One of the key questions around LPMO action is why many organisms have multiple LPMO genes.[2] To answer this question will require structure-function studies of multiple LPMOs from well-characterized organisms. This paper describes the first LPMO structure from the fungus *Phanerochaete chrysosporium*, an organism that has a repertoire of more than ten LPMO genes. We elucidate the product distribution of an LPMO enzyme directly from a biomass substrate. We have, for the first time, conducted molecular dynamics simulations of these systems on the cellulose surface, and revealed molecular-level details of the enzyme-substrate interaction.

[1] G. Vaaje-Kolstad et al. *Science* **2010**, *330*, 219-222.
[2] D. Floudas et al. *Science* **2012**, *336*, 1715-1719.

Expression, structure and cellulase activity of the cellobiohydrolase Cel7A from the fungus *H. grisea* var. *thermoidea*

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Glycoside hydrolase family 7 (GH7) cellobiohydrolases (CBH) play a key role in biomass recycling in nature. The thermostability of the enzyme is an important parameter for industrial utilization. In this study, Cel7 enzymes from different fungi were expressed in a fungal host and assayed for thermostability, with *Hypocrea jecorina* Cel7A as reference. The most stable of the homologs, *Humicola grisea* var. *thermoidea* Cel7A (*Hgt*Cel7A), exhibits 10 °C higher melting temperature, showed 4-5 times higher initial hydrolysis rate than *H. jecorina* Cel7A on phosphoric acid swollen cellulose, and the best performance of the tested enzymes on pretreated corn stover at elevated temperature. The crystal structure of the *H. grisea* var. *thermoidea* Cel7A catalytic module is similar to that of other GH7 CBHs.[1]

[1] M. Haddad Momeni et al. *Acta Crystallogr., Sect. D* **2014** *(in press)*
[2] B.C. Knott et al. *J. Am. Chem. Soc.* **2014**, *136*, 321-329.

Poster IAF-12

Poster IAF-13

Regioselectivity of α-galactosidase from *T. maritima* in hydrolysis and transglycosylation reactions

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Glycoside hydrolases are known for their hydrolytic activity towards different types of glycosidic linkages and wide regioselectivity. α-galactosidase *Tm*GalA from *Thermotoga maritima* belongs to glycoside hydrolase family 36. Like other retaining glycoside hydrolases, *Tm*GalA shows transglycosylation activity and is of potential interest for synthesis of valuble galacto-glycoconjugates. We have studied the regioselectivity for both hydrolysis and transglycosylation and find in both cases a preference for the α-1,3-glycosidic linkage. A novel method for determination of enzyme kinetic parameters based on step-by-step hydrolysis of labelled oligosaccharides revealed significant impact of non-enzymatic mutarotation on the hydrolysis reaction. We also show that the alpha-anomer of galactose is a much stronger inhibitor than the beta-anomer. Therefore, mutarotation from the α-anomer, which is the product of the hydrolytic reaction, to the β-anomer, needs to be taken into consideration during the course of hydrolysis experiments. We propose a mathematical model that accounts for mutarotation in the evaluation of enzyme kinetic studies.

LC-QTOF-MS based metabolomics for dietary exposure biomarker discovery and validation

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It is well-known that diet has strong effects on human health and influences the risk of developing type 2 diabetes (T2D).[1] Most evidence comes from epidemiological studies where food intake is typically based on self-reporting measurements such as food frequency questionnaires. These methods are prone to relatively large measurement errors that may mask true diet-disease relationships. Dietary exposure biomarkers, i.e. compounds specific for certain foods or dietary patterns or their metabolites, measured in biological body fluids may be used to overcome the problems.[2-4] The aim of this study is to discover and validate dietary exposure markers and to find prediction biomarkers of T2D in men and women. An untargeted LC-QTOF-MS based metabolomics approach is currently applied to develop and validate novel dietary exposure biomarkers that could be applied for assessment of the risk of developing T2D in a nested case-control study.

[1] V. Salomaa et al. *Biomarkers of Diabetes* **2010**, *5*, 1-8.
[2] V.E. Hedrick et al. *Nutr. J.* **2012**, *11*, 109.
[3] A. O'Sullivan et al. *Am. J. Clin. Nutr.* **2011**, *93*, 314-321.
[4] L. Penn et al. *Genes Nutr.* **2010**, *5*, 205-213.

Poster IAF-14

Poster IAF-15

Rational design, synthesis & enzyme-substrate structures of fluorogenic substrates for family 6 glycoside hydrolases

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Methylumbelliferyl-β-cellobioside (MUF-G2) is a convenient fluorogenic substrate for certain β–glycoside hydrolases (GH). However, hydrolysis of the aglycone is poor with GH family 6 enzymes (GH6), despite strong binding. Prediction of the orientation of the aglycone of MUF-G2 in the +1 subsite of *Hypocrea jecorina* Cel6A by automated docking suggested umbelliferyl modifications at C4 and C6 for improved recognition. Four modified umbelliferyl-β-cellobiosides ClMUF, ClF_3MUF, PhUF, and ClPhUF were synthesized and tested with GH6, GH7, GH9, GH5 and GH45 cellulases. The 4-phenyl substitution drastically reduced the fluorescence intensity of the free aglycone, while ClMUF-G2 could be used for determination of k_{cat} and K_M for *H. jecorina* Cel6A and *Thermobifida fusca* Cel6A. Crystal structures of *H. jecorina* Cel6A D221A mutant soaked with the MUF-, ClMUF- and ClPhUF-β-cellobioside substrates show that the modifications turned the umbelliferyl group 'upside down', with the glycosidic bond better positioned for protonation than with MUF-G2.[1]

[1] M. Wu et al. *FEBS J.* **2013**, *280*, 184-198.

GC/MS method for determination of alkylresorcinols in human subcutaneous adipose tissue biopsy samples

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Whole grain foods are rich in vitamins, minerals, dietary fiber and various phytochemicals. Epidemiologic studies have shown protective associations between whole grain intake (48-80 g/d) and risk of developing type 2 diabetes, cardiovascular disease and some cancers in humans. Most of these studies rely on self-reported data which may be subject to large measurement errors. A biomarker of whole grain intake may be used for more objective intake estimation. Alkylresorcinols (ARs) are a group of phenolic lipids found in the bran part of wheat and rye grains but not in refined cereal products or in other commonly consumed foods. ARs are absorbed by humans. Plasma and their metabolites in the urine have been suggested and evaluated as biomarkers of whole grain wheat and rye intake under different conditions. The apparent half-life of ARs in plasma is short (5h) and 24h urine collections are rarely collected in prospective cohort studies. In epidemiological studies, long term intake of whole grain foods is of main interest and long-term biomarkers are therefore wanted. The new GC-MS method presented can be used for rapid analysis of ARs in small amount of adipose tissue from needle biopsy at adequate precision.

Poster IAF-16

Poster IAF-17

Activity of cytochrome P450 in the different lobes of the porcine liver

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Due to limited supply of human livers for research, pig tissue and hepatocytes has been suggested as an attractive alternative when studying human drug metabolism by cytochrome P450 (CYP450). In order to suggest the porcine liver lobe which resembles the human liver the most with respect to CYP450 activity, we investigated lobe differences in the activity of individual CYP450 isoforms. Livers from six female pigs (63.0 ± 3.6 kg; crossbreeds between Duroc boars and Landrace x Yorkshire dams) were removed immediately after slaughter. The entire liver was oriented with the visceral surface facing upwards and the four lobes identified: the left/right lateral/medial lobes. Then ca. 5 g of liver tissue was punched out from the middle of each lobe using a hollow metal cylinder. Tissue was immediately frozen in liquid nitrogen and stored at -80 °C until microsome preparation. CYP450 activities were determined by incubating the liver microsomes with one of the following selective substrates: ethoxyresorufin, methoxyresorufin, coumarin, tolbutamide, *p*-nitrophenol, and benzyloxyresorufin. The CYP450 activities did not significantly differ between the different lobes. This implies that, though there is great variation between individual pigs, any part of the porcine liver are equally useful as model tissue.

Structure and function of fimbrial polyadhesins

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Successful establishment of infection by bacterial pathogens requires adhesion to host cells, colonization of tissues, and cellular invasion. Most Gram-negative pathogenic bacteria use the chaperone/usher (CU) pathway to assemble, on their surface, large adhesive proteinaceous structures called fimbriae or adhesive pili. Fimbriae are immunogenic so they can be high-profile vaccine candidates.[1] Structural and ligand binding information can enhance vaccine and antimicrobial drug development efforts. Many CU fimbriae act as mono-adhesins, using only one specialized subunit to attach to a host cell receptor. Recently, our group demonstrated that a large class of CU fimbriae could use major polymeric subunits for attachment, acting as polyadhesins.[2] To elucidate this novel mechanism of attachment, we studied isolated subunits of CU polyadhesins and binding determinants of host cell receptors. X-ray crystallography was used as the main method to visualize the fimbriae-receptor interactions. To characterize the binding we use surface plasmon resonance, isothermal titration calorimetry, and tryptophan fluorescence quenching. Here, we report studies with several types of fimbriae (CS6, AAF-1 and Myf) from *E. coli* and *Yersinia enterocolitica*.

[1] A. Zavialov et al., *FEMS Microbial Rev.* **2007**, *31*, 478-514.
[2] S.P. Roy et al., *Mol. Microbiol.* **2012**, *86*, 1100-1115.

Poster IAF-18

Poster FFN-01

New antibiotics from nature: SLU/Medivir collaboration

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Antibiotic resistance is increasing – new antibiotics are urgently needed. The challenges to antibacterial discovery have kept the output of novel antibacterial drug classes at extraordinarily low levels over the past 50 years and rational drug design of new compounds has failed.

International expert organizations, such as Infectious Diseases Society of America (IDSA) and British Society for Antimicrobial Chemotherapy are now proposing a return to nature as a place to find new antibiotics. As an example the IDSA 10 × ’20 initiative committed to the need to develop ten new antibacterial drugs by 2020.

A collaboration between SLU and Medivir started in August 2012 with the primary objective to discover and develop new antibiotics from natural sources active against bacteria resistant to present therapies.

[1] IDSA *Clin. Infect. Dis.* **2010**, *50*, 1081-1083.

Poster FFN-02

Carbohydrate quality of products prepared using barley flour with different dietary fibre and starch composition

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Despite the acknowledged health benefits of dietary fibres a majority of people has a dietary fibre intake below the recommended. One reason is the high consumption of products made from white wheat flour which contain low amount of dietary fibre. These should be replaced with products containing more dietary fibre, for example products made from barley flour which naturally has a higher amount of dietary fibre and especially of β-glucan which is known to lower cholesterol levels.

This project studies the effects of different carbohydrate compositions in cereals and cereal structures on end product quality of cereal foods. Five barley varieties with different dietary fibre and starch composition together with a control are used in this project. Two food products have been produced, one bread where the slow process allows endogenous enzymes to act on the dietary fibre polysaccharides, and one extruded product made with high temperature and high shear. Both products can be evaluated from 2 different aspects: How does starch and fibre composition affect processing and product properties? How does processing affect starch and fibre in the different barleys? The influence of processing on carbohydrate quality is studied in detail with a number of chemical analyses.

Poster FFN-03

Optimized FDR estimation in proteomics by using *p*-value scoring

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All search algorithms for mass spectrometry based proteomics report some quantity that aims at describing how good an individual protein identification result is. These quantities are referred to as scores. A good score can however never guarantee that a result is true, since false results can sometimes yield a good score by chance. It is therefore desirable that a score reflects the statistical risk that an individual result is false – *i.e.* the significance level (*p*-value). In a large proteomics data set with a substantial portion of low quality spectra it is likely to obtain some false results that yield good scores or *p*-values by chance. A false discovery rate (FDR) calculation is assumed to measure the risk that this occurs for a given dataset and score threshold.

Our simulation with different algorithms and using datasets with *realistic* synthetic fragment spectra with different numbers of fragments and precursor ion masses and searching in both real and decoy (reversed) sequence collections, allowed us to monitor the real distribution of true and false results and to compare this with the predictions by FDR estimations. We demonstrate that the scoring method influences the deviation between real and estimated FDR calculations.

Chemical characterization of secondary metabolites of plant growth-promoting *Serratia* spp

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Some species of Gram-negative rhizobacteria of the genus *Serratia* have been found to be antagonistic to the phytophatogen *Rhizoctonia solani*, while being beneficial to plant growth. The aim of this project is to discover antifungal secondary metabolites produced by species of *S. plymuthica* and *S. proteamaculans* that may explain the inhibition of *R. solani*.

Agar plugs containing the diffusible metabolites in the interaction zone between the fungus and the bacterium in dual cultures were excised at regular intervals and the metabolites were analyzed by full scan LC-MS. Several secondary metabolites produced by *Serratia plymuthica*, such as pyrrolnitrin, prodigiosin, serratamolides and siderophores, known for their involvement in antifungal activity, were detected.[1] None of these, however, was significantly up-regulated in the samples where the bacteria were co-inoculated with the fungus, compared to levels in single cultures. Some unknown compounds, detected only in the interaction zones, will be further isolated and identified.

[1] L.M. Petersen et al. *Can. J. Microbiol.* **2013**, *59*, 627-640.

Poster FFN-04

Poster FFN-05

Microstructure of whole grain rye products and its impact on *in vitro* digestion

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Overconsumption of foods is a strong contributor to obesity and its related disorders, the fifth leading cause of deaths globally.[1] Development of tailored foods could be one way to address the problem. Process induced changes in microstructure and composition may be of importance for the rheological properties and particle size distribution of the digesta, which could influence absorption kinetics of nutrients.[2] This could influence postprandial responses and perceived satiety.[3] The overall aim is to elucidate if and how microstructural features contribute to beneficial postprandial responses.

In general, the rye products gave higher digesta viscosites than wheat ones. The digested porridge gave the highest digesta viscosity. The digested rye products also contained larger particles than the wheat products. There were however, significant differences between the rye products as well with the digesta of extruded product containing the smallest particles.

[1] E. Wirfält et al. *Food Nutr. Res.* **2013**, *57*: 20523
[2] L. Marciani et al. *Am. J. Physiol. Gastrointest. Liver Physiol.* **2001**, *280*, G1227–1233.
[3] C. De Graaf et al. *Am. J. Clin. Nutr.* **2004**, *79*, 946–961.

Uptake of dioxins and polycyclic aromatic compounds from soil by zucchini (*Cucurbita pepo*)

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Zucchini belongs to the *Cucurbita* genus, and it is known to accumulate organic pollutants from soil. In this study, zucchini (*Cucurbita pepo*) was grown on soil from two contaminated sites. One site was contaminated with polychlorinated dibenzo-*p*-dioxins and dibenzofurans, and the other site with polycyclic aromatic compounds (PACs). PACs include the well-known soil pollutants polycyclic aromatic hydrocarbons (PAHs), but also more polar PACs such as the oxy-PAHs. The oxy-PAHs are produced in the same processes as PAHs, but can also be formed when PAHs degrade in the environment. The contaminants included in this study were the seventeen 2,3,7,8-substituted dioxins, 16 PAHs and 11 oxy-PAHs, thus covering substances that differ substantially in hydrophobicity and other physicochemical properties. The aim of the study was to determine the uptake by zucchini and to investigate if the uptake varied between the different contaminants and between the different soils. We also investigated to what extent the uptake correlated to soil parameters, for instance the content of organic carbon and black carbon.

Poster FFN-06

Poster FFN-07

Metabolic response of the wood-decomposing fungus *Granulobasidium vellereum* to seven competing fungi

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The wood decomposing fungus *Granulobasidium vellereum* has been shown to produce a multitude of different sesquiterpenes.[1,2] The large number of compounds might indicate an unspecific enzymatic machinery which allows the fungus to produce a large variety of biosynthetically closely related compounds, of which a only a few are of importance for the interaction with competing species.

To test which of the secondary metabolites from *G. vellereum* that are important for the interaction with other fungi, dual culture fungus-fungus interaction systems were established between *G. vellereum* and seven selected fungal species. The samples were analyzed using LC-HRMS. PCA analysis of the data showed that some of the secondary metabolites of *G. vellereum* were up-regulated in the interaction zone between the fungi. Some of the up-regulated metabolites could be identified as previously isolated from *G. vellereum*.

[1] Nord, C.L. et al. *Phytochemistry* **2013**, *90*, 128-134.
[2] Nord, C.L. et al. *Phytochemistry* **2014**, *102*, 197-204.

Development of a sustainable method for mycotoxin prevention in cereals

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Fusarium head blight (FHB) is a re-emerging disease in small grain cereals in Sweden, as well as worldwide. It impairs both the grain yield and the quality. Most serious consequence is the contamination of grain with *Fusarium* mycotoxins that are severe threat to humans and animals. We have studied the possibility to prevent the disease and consequent myxotoxin production using our biocontrol agents (BA) The bacteria were recently isolated from harsh environments in Israel and Arizona and have been shown by us to be excellent plant growth promoting rhizobacteria (PGPR) due to the production of novel biologically active compounds.[1,2] One of the isolates *Paenibacillus polymyxa* A26 was very efficient against *Fusarium* spp. The A26 genomic sequence reveals that it harbours nine giant gene clusters directing synthesis of bioactive peptides and polyketides by modularly organized megaenzymes.

[1] Timmusk S. et al. *PLOS ONE* **2014** *(in press)*
[2] Timmusk S. et al. *PLOS ONE* **2011**, *6*, e17968.

Poster FFN-08

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Notes

time	Tuesday, August 19	Wednesday, August 20	Thursday, August 21
8.20		**Plenary 2: Albert Mihranyan**	**Plenary 4: Maud Langton**
8.40			
9.00			
9.20		Anna Rising	Kristine Koch
9.40		Mats Sandgren	Jana Pickova
10.00		Gulaim Seisenbaeva	Thomas Moritz
10.20		*coffee break*	*coffee break*
10.40		Torleif Härd	Folke Sitbon
11.00		Volkmar Passoth	Marie Bengtsson
11.20		Meritxell Gros-Calvo	Göran Birgersson
11.40		Mirco Bundschuh	*research strategy discussion & closing of the conference*
12.00		*lunch (not included)*	
12.20			
12.40			
1.00	*opening ceremony*		
1.20	**Plenary 1: Gordon Brown**	**Plenary 3: Mikael Lindgren**	
1.40			
2.00			
2.20	Jon-Petter Gustafsson	Geoffery Daniel	
2.40	Maja Larsson	Fabrice Magne	
3.00	*poster session & coffee break*	*poster session & coffee break*	
3.20			
3.40			
4.00	Dan Berggren-Kleja	Corine Sandström	
4.20	Ingmar Persson	Karin Wiberg	
4.40	Elin Lavonen	Stephan Köhler	
5.00	Jens Fölster	Roksana Wierzbicka	
5.20	*day 1 closing remarks*	*day 2 closing remarks*	
6.30		*conference dinner (until 10 pm)*	

General information

Each **plenary talk** is scheduled to last **45 minutes + 10 minutes** of questions

Each **oral presentation** is scheduled to last **15 minutes + 5 minutes** of questions

Poster presentations should be put up before 3 p.m. on Tuesday and removed no later than noon on Thursday.

Wednesday lunch is **not included** in the conference.

The **conference dinner** will be held at **Ultunarestaurangen.**

Schedule changes, if any, **will be announced** at the beginning of each presentation block.