KBC DAYS 2018

6-7 November, KBC-building

Programme - Abstracts - Research Infrastructures

UMEÅ UNIVERSITY
SLU
KBC on focus environment
KBC Chemical Biological Centre
Umeå University/SLU
www.kbc.umu.se/english

Tuesday, 6th November

8.30 **Registration and poster mounting**

SESSION 1
Chairperson: Stefan Jansson

9.00 **Opening of the KBC Days 2018**
Hans Adolfsson
Vice chancellor, Umeå University

9.10 **tba**
Katrine Riklund
Pro-Vice-Chancellor, Umeå University

9.25 **Welcome**
Stefan Björklund
Scientific Coordinator of KBC

9.30 **tba**
Oliver Billker
Department of Molecular Biology and The Laboratory for Molecular Infection Medicine Sweden (MIMS), Director of MIMS

10.30 *Coffee break*

SESSION 2: PRESENTATIONS FROM THE MEDICAL BIOLOGY CENTRE (MBC)
Chairperson: Elisabeth Sauer-Eriksson

11.00 **More than early development of the eye and olfactory epithelium**
Lena Gunhaga
Umeå Centre for Molecular Medicine (UCMM)

11.20 **AMPK activator O304 - a novel type 2 diabetes and obesity drug**
Helena Edlund
Umeå Centre for Molecular Medicine (UCMM)

11.40 **Imaging the pancreas in diabetes - optical techniques to study islet function and disease dynamics**
Ulf Ahlgren
Umeå Centre for Molecular Medicine (UCMM)

12.00 **Human sensorimotor control: from single sensory neurons to complex adaptive behavior**
Michael Dimitriou
Department of Integrative Medical Biology (IMB)

12.20 *Lunch*

SESSION 3: PRESENTATIONS FROM THE MEDICAL BIOLOGY CENTRE (CONTINUED)
Chairperson: Andrei Chabes

13.20 **How inhibition gets exciting – Chloride ions in control of brain activity**
Staffan Johansson
Department of Integrative Medical Biology (IMB)

13.40 **Exploring brain circuits in the healthy and diseased brain at high spatio-temporal resolution**
Paolo Medini
Department of Integrative Medical Biology (IMB)

14.00 **Neural guidance in development and disease**
Sara Wilson
Department of Integrative Medical Biology (IMB)

14.20 *Coffee break*

SESSION 4
Chairperson: Christiane Funk

14.50 **KBC during the last and the coming year**
Stefan Björklund
Scientific Coordinator of KBC

15.10 **Sustainable Chemistry**
Klaus Kümmerer
Institute for Sustainable and Environmental Chemistry, Leuphana University, Lüneburg, Germany

15.55 **Disarming of drug resistance in *Mycobacterium tuberculosis***
Fredrik Almqvist
Department of Chemistry

16.15 **PRESENTATIONS FROM MIDTERM PHD STUDENTS**
(2 minutes each)

Characterization of adventitious root formation in Norway spruce
Sanaria Alallaq
Umeå Plant Science Centre (UPSC), Department of Plant Physiology

Putative b-galactosidases linked to a loss of anisotropic growth in *Arabidopsis* roots
Pieter Nibbering
UPSC, Department of Forest Genetics and Plant Physiology

PIRIN2 suppresses non-cell-autonomous lignification in *Arabidopsis* xylem
Bernadette Sztojka
UPSC, Department of Plant Physiology

Alternative assessment of hazard chemicals combining in silico tools with multicriteria decision analysis (MCDA): a case study of decabromodiphenyl ether (decaBDE) alternatives
Ziye Zheng
Department of Chemistry

How do sugars regulate flowering? Is epigenetic regulation the missing link?
Noemi Skorzinski
UPSC, Department of Plant Physiology

NEP activity is essential for the expression of plastid photosynthesis genes during chloroplast development
Yan Ji
UPSC, Department of Plant Physiology

Outlier detection in neural networks - Chemometrics meets deep learning
Rickard Sjögren
Computational Life Science Cluster (CLiC), Department of Chemistry

Influence of cook stove technology and fuels on particle emissions - A detailed characterization on physical and chemical properties
Robert Lindgren
Thermochemical Energy Conversion Laboratory (TEC-Lab), Department of Applied Physics and Electronics

16.35 *Smoothies and fruits*

16.40 POSTER PRESENTATIONS

The midterm PhD students and KBC platforms/ infrastructures present their posters in the KBC Cafeteria (printed and digital presentations)

18.00 *Dinner with Live Music from Second Hand band*

Wednesday, 7th November

SESSION 5
Chairperson: Sebastian Diehl

8.50 **Infrastructure from the far side**
Jonathan Gilthorpe
Department of Pharmacology and Clinical Neuroscience

9.00 **Presenting Umu research infrastructures - infrastructure portal at Umu.se**
Kristoffer Lindell
Project leader, Planning Office

9.15 **The physics workshop**
Isak Silander
Mechanical workshop at the Department of Physics

NEW FACULTY MEMBERS AND AWARD RECIPIENTS AT KBC

9.25 **Mitochondrial DNA – our overlooked genome**
Paulina Wanrooij
Department of Medical Biochemistry and Biophysics

9.45 **Modeling the evolutionary origins of multicellularity**
Eric Libby
Department of Mathematics and Mathematical Statistics

10.05 **Robustness and modularity of gene regulation in development and disease**
Andreas Hörnblad
Umeå Centre for Molecular Medicine (UCMM)

10.25 **Coffee and presentation of the KBC Poster Award 2018**

SESSION 6: NEW FACULTY MEMBERS AND AWARD RECIPIENTS AT KBC (CONTINUED)
Chairperson: Natuschka Lee

10.50 **The Spiderhunt – combining citizen science with basic research**
Jerker Fick
Department of Chemistry

11.10 **Immunomodulatory properties of bacterial genotoxins: from killing to subversion of host responses**
Teresa Frisan
Department of Molecular Biology

11.30 **Swelling of graphite/graphene oxides in polar solvents**
Alexandr Talyzin
Department of Physics

11.50 **Genomes in space and time**
Per Stenberg
Department of Molecular Biology and Department of Ecology and Environmental Sciences

12.10 **Bacterial conjugation via Type 4 Secretion Systems**
Ronnie Berntsson
Department of Medical Biochemistry and Biophysics and Wallenberg Centre for Molecular Medicine (WCMM)

12.30 *Lunch*

13.30 **GUIDED TOURS ORGANISED BY THE KBC INFRASTRUCTURES**
(Sign up for the tours at the registration desk)

- ***Biochemical Imaging Centre Umeå, BICU (Irene Martinez Carrasco)***
- ***Biogeochemical Analytical Facility, BAF (Anders Jonsson)***
- ***Chemical Biology Consortium Sweden, CBCS Umeå (former LCBU) (Stina Berglund Fick)***
- ***NMR Core Facility (Jürgen Schleucher, Gerhard Gröbner)***
- ***Proteomics Core Facility (Thomas Kieselbach)***
- ***Swedish Metabolomics Centre Umeå (Annika Johansson)***
- ***Umeå Core Facility for Electron Microscopy, UCEM (Linda Sandblad)***
- ***Vibrational Spectroscopy Core Facility, ViSp (András Gorzsás)***
- ***X-ray Crystallography Platform and Protein Expertise Platform, PEP (Uwe Sauer, Mikael Lindberg)***
- ***X-ray Protoelectron Spectroscopy Platform, XPS (Andrey Shchukarev)***
- ***The Trace Analysis Platform, TAP (Per Liljelind)***

Poster Abstracts - Midterm PhD students

P1

Characterization of adventitious root formation in Norway spruce

Sanaria Alallaq[1], Abdellah Lakehal[1], Federica Brunoni[1,2], Ondrej Novák[3] and Catherine Bellini[1,4]

[1]Umeå Plant Science Centre, Department of Plant Physiology, Umeå University, 90187 Umeå, Sweden

[2]Umeå Plant Science Centre, Department of Forest Genetics and Plant Physiology, SLU, 90183 Umeå, Sweden

[3]Centre of the Region Haná for Biotechnological and Agricultural Research, Palacký University, Olomouc, Czech Republic

[4]Institut Jean-Pierre Bourgin, INRA, AgroParisTech, CNRS, Université Paris-Saclay 78000 Versailles, France

The root system of a plant is composed of the primary, lateral and adventitious roots (ARs). Adventitious roots form from stem or leaf derived cells. Adventitious rooting is an essential step in artificial vegetative propagation of plants. In horticulture, agriculture and forestry, vegetative or clonal propagation is widely used to multiply elite genotypes obtained in breeding programs or selected from natural populations. During the last decade, using the model plant *Arabidopsis thaliana* we showed that AR initiation is regulated by a transcriptional regulatory modules acting at the crosstalk of the auxin and jasmonate signaling pathways. Our aim is to take advantage of the knowledge acquired so far in *Arabidopsis* and go a step further in the understanding of key regulatory genetic factors controlling AR initiation in *P. trichocarpa* (easy-to-root) and *P. tremula* x *P. tremuloides* (difficult-to-root) species, by means of different approaches and we would like to adopt an evolutionary point of view and analyze how our knowledge translates to Norway spruce (*Picea abies*), which is the economically most important tree in Sweden. In this poster we will present the effect of different light regimes on adventitious root formation on hypocotyls of Norway spruce (*Picea abies*) de-rooted seedlings, and the consequences the different light conditions have on the hormone homeostasis. We also performed an anatomical characterisation of the different stages of development of AR in hypocotyls kept in different light conditions which will presented on this poster.

P2

Putative β-galactosidases linked to a loss of anisotropic growth in arabidopsis roots

Pieter Nibbering[1], Bent L. Petersen[2], Peter Ulvskov[2], Totte Niittylä[1]

[1]Department of Forest Genetics and Plant Physiology, Umeå Plant Science Centre, Swedish University of Agricultural Sciences, 901 83 UMEÅ

[2]Department of Plant Glycobiology, University of Copenhagen, DK-1871 Frederiksberg C, Denmark

In an effort to identify genes involved in arabinogalactan (de)glycosylation in *Arabidopsis*, we identified two glycoside hydrolase genes which cause sugar induced root swelling when mutated. The genes were named Root Swelling Phenotype (RSP). The RSP proteins are part of a glycoside hydrolase family, which is conserved between prokaryotes, fungi and plants. The bacterial and fungal RSP related proteins have been shown to have xylosidase, arabinase or galactanase activity, and phylogenetic analysis suggested that the RSP proteins may be β1,3 galactanases. These structures are only found in the highly glycosylated arabinogalactan proteins (AGPs), pectin and possibly in cytosolic heteroglycans involved in starch degradation. Galactan containing polymers are synthesized in the Golgi and in accordance with this the RSP-YFP fusion proteins were localized to the Golgi apparatus. Furthermore the sugar induced root swelling of the *rsp* double mutant coincided with an increase in arabinose and galactose. Preliminary results with specific antibodies suggest that this increase is related to altered AGP side chain composition in the rsp null mutant. Currently, I am analyzing the cell wall glycoprotein fraction in more detail and characterizing the in vitro activity of purified RSP proteins to define their substrate specificity.

P3

PIRIN2 suppresses non-cell-autonomous lignification in *Arabidopsis* xylem

Bo Zhang[1], Bernadette Sztojka[1], S. Escamez[1], P. Cs. Miskolczi[2], R. Vanholme[3,4], M. Hedenström[5], A. Gorzsas[5], R. P. Bhalerao[2], W. Boerjan[3,4], H. Tuominen[1]

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[2]Umeå Plant Science Center, Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, S-901 83 Umeå, Sweden

[3]Ghent University, Department of Plant Biotechnology and Bioinformatics, Technologiepark 927, 9052 Gent, Belgium

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PIRINs (PRN) are highly conserved cupin domain containing proteins, which have been implicated in numerous biological processes, including transcriptional co-regulation in mammals, but that are not extensively studied in plants. The *PRN* gene family was previously identified as a potential novel regulator of lignification in the developing tracheary elements in *Zinnia elegans* cell cultures (Pesquet et al., 2013).

In *Arabidopsis thaliana* histochemical GUS assay revealed the very specific expression of the homologous *PIRIN2 (PRN2)* in the xylem cells that were located next to xylem vessel elements. Cell wall chemistry analysis of two *prn2* knock-out mutants demonstrated slightly increased lignin content and a significant increase in the ratio of the S- to the G-type lignin compared to the wild-type, which correlated with changes in expression of lignin biosynthetic genes. Overproduction of PRN2 resulted in the opposite phenotype. Fourier transform infrared spectroscopy and Raman microspectroscopy showed that PRN2 modulates cell wall chemistry of the neighbouring vessel elements and fibers, hence contributing to their lignification in a non-cell-autonomous manner. Interaction assays resulted in the identification of the chromatin modifying E3 ubiquitin ligase HISTONE H2B MONOUBIQUITINATION2 (HUB2) as an interactor of PRN2. *HUB2* is not expressed in vessel elements, but Raman analysis revealed that HUB2 suppresses the accumulation of G-type lignin in the vessel cell walls. Altogether, the results suggest that PRN2 regulates, together with HUB2, lignification in a non-cell-autonomous fashion by regulating the expression of lignin biosynthetic genes.

Reference:

Pesquet, E., Zhang, B., Gorzsás, A., Puhakainen, T., Serk, H., Escamez, S., Barbier, O., Gerber, L., Courtois-Moreau, C., Alatalo, E., Paulin, L., Kangasjärvi, J., Sundberg, B., Goffner, D., and Tuominen, H. (2013). Non-cell-autonomous postmortem lignification of tracheary elements in *Zinnia elegans*. The Plant Cell 25, 1314-1328.

P4

Alternative assessment of hazard chemicals combining *in silico* tools with multicriteria decision analysis (MCDA) - a case study of decabromodiphenyl ether (decaBDE) alternatives

Ziye Zheng[1], Gregory Peters[2,3], Hans Peter H. Arp[4,5], Patrik L. Andersson[1]

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[2]Division of Environmental Systems Analysis, Chalmers University of Technology, SE-412 96 Göteborg, Sweden
[3]Department of Civil and Environmental Engineering, University of New South Wales, Sydney, Australia
[4]Department of Environmental Engineering, Norwegian Geotechnical Institute, Ullevaal Stadion, NO-0806 Oslo, Norway
[5]Department of Chemistry, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Alternative assessment is applied for minimizing the risk of replacing a hazardous chemical with another problematic, hazardous chemical. Ideally, such alternative assessments would be based on high quality experimental data, for all relevant hazard endpoints. Such data are however usually unavailable, especially for newly produced or proposed alternatives. In such cases, obtaining *in silico* data is the only approach to fill in data gaps while the quality of such data is generally less certain. An additional concern is how to reach a decision based on uncertain *in silico* data across multiple endpoints.

To address these problems, this study explored the use of different multicriteria decision analysis (MCDA) methods within an alternative assessment framework. For this, sixteen alternatives to a widely used flame retardant - decabromodiphenyl ether (decaBDE) - were considered as the case chemicals. This study also discussed what endpoints should be included for assessing the hazard. The hazard endpoints include not only persistence (P), bioaccumulation potential (B) and toxicity (T) which are generally considered by existing alternative frameworks, but also the mobility in water (M) which is fairly recent, and to our knowledge this is the first study to include M within an alternative assessment. Experimental data were collected from free-access databases and *in silico* data were calculated by open-source software or platforms.

As expected, the data distribution of experimental data was uneven and large data gaps existed. *In silico* data were calculated for five P criteria, one B criterion, 13 T criteria and one M criterion and were able to address these data concerns. Three MCDA strategies were tested in this case study: heat map, MAUT and ELECTRE III. These different MCDA strategies led to different conclusions on some of the chemicals. However, in aggregate the results of these three MCDA approaches provided meaningful insights in how to use *in silico* data to make an appropriate final-decision strategy for a selection of alternatives. The results also point out that the potentially best alternative can be different depending on considered exposure pathway, which stresses the importance of exposure by the different final-score approaches (PBT, PMT or PBMT).

P5

How do sugars regulate flowering? Is epigenetic regulation the missing link?

Noemi Skorzinski[1], Jathish Ponnu[2,3], Tobias Langenecker[2], Markus Schmid[1]

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[2]Dept. of Molecular Biology, Max Planck Institute for Developmental Biology, Tübingen, Germany

[3]Present address: Botanical Institute, University of Cologne, Cologne, Germany

One way for plants to maximize their reproductive success is to optimise timing of flowering. Thus, in most plant species, flowering time is not deterministic but can be adjusted in response to environmental and endogenous signals. Environmental signals, e.g. daylength (photoperiod) and temperature, indicate if it is the right season to flower, whereas endogenous factors, e.g. age, hormones and nutritional status, inform the plant if it is able to support the energy-demanding processes of flowering and seed production. The different regulatory signals are integrated in a network of interconnected pathways, ensuring plasticity in timing of flowering.

An important regulator of flowering time in *Arabidopsis thaliana* is carbohydrate availability, which is signalled through trehalose 6-phosphate (Tre6P). Tre6P is synthesized by TREHALOSE-PHOSPHATE SYNTHASE 1 (TPS1) and *tps1* loss-off-function mutants have been shown to be extremely late flowering and sterile. Tre6P regulates flowering in two ways: it inhibits the SnRK1 protein kinase complex, which otherwise activates several genes that supress flowering, and it modulates flowering via the photoperiod and age pathway. However, surprisingly little is known about the molecular mechanisms connecting carbohydrate concentration and induction of flowering.

To identify new components that connect carbohydrate signalling and flowering, we mutagenized the late flowering *tps1-2* mutant with EMS. Screening M2 mutants for restored flowering and seed set, we found close to 100 suppressor mutations. Among those suppressors, we identified multiple alleles in two genes that encode subunits of the SnRK1 protein complex. Three other candidate genes encode epigenetic regulators involved in histone modifications. None of the candidate genes had so far not been implicated in the TPS1/Tre6P pathway.

We are currently performing several experiments to test if TPS1/Tre6P regulates flowering through epigenetic regulation. These include analysis of higher order mutant of *tps1-2* and mutants of the candidate genes, as well as ChIP-seq and RNA-seq to compare the epigenetic landscape and its effect on gene expression between Col-0 wildtype plants and the *tps1-2* mutant.

P6

NEP activity is essential for the expression of plastid photosynthesis genes during chloroplast development

Louise Norén[1], Yan Ji[1] and Åsa Strand[1]

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The plastid-encoded genes of higher plants are transcribed by at least two types of RNA polymerases, the nuclear-encoded plastid RNA polymerase (NEP) and the plastid-encoded RNA polymerase (PEP). In mature photosynthesizing leaves, the vast majority of the genes are transcribed by PEP but during chloroplast development the division of labour between NEP and PEP is unclear. RNAseq analysis demonstrated that at least 50% of the plastid transcriptome is rapidly induced in response to light. Analysis of mutants with deletions of sigma factor 2 and 6, respectively, demonstrated that the early light induction observed for the plastid encoded photosynthesis genes was not affected in the *sig* mutants. This suggests that NEP is the main RNA polymerase during this time period. In addition, similar to the plastid encoded genes, expression of the NEP gene, *SCABRA3* was rapidly induced by light. We show that this induction was abolished in the *bzip16bzip68gbf1* triple mutant, and as a consequence, more than 90% of the plastid-encoded genes showed significantly reduced expression levels in response to light compared to wild type. In addition, development of the thylakoid membrane and chlorophyll accumulation were impaired in the *bzip* triple mutant. Thus, bZIP16, bZIP68 and GBF1 are required for light induced expression of *SCABRA3*, plastid transcription and proper chloroplast development during the early light response. Our results suggest that NEP activity is essential for expression of the plastid encoded photosynthesis genes during the early phase of chloroplast development.

P7

Outlier Detection in Neural Networks - Chemometrics Meets Deep Learning

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Deep learning has revolutionized the fields of computer vision, artificial intelligence, natural language processing, and rely on a type of model called deep artificial neural networks. Even though deep neural networks are powerful models, their predictions fail completely when they encounter data that is dissimilar to data used for model fitting, so called outliers. The most alarming part is that the models give no warning. Adoption of deep learning in safety-critical systems raise the need for understanding what deep neural networks do not understand, and knowing when they fail. Several methodologies to estimate uncertainty in deep neural networks have been proposed, but these impose constraints on how the models are used.

Chemometrics has long been used in process manufacturing monitoring, in which outliers are a well-known and solved problem. Chemometrics rely on linear latent variable methods such as Principal Component Analysis (PCA) or Partial Least Squares (PLS) regression. Linear latent variable models allow detection of outliers by simply measuring distances, either within the model or to the model. However, these principles cannot be directly applied in the context of deep neural networks.

We present an assumption-free method allowing deep neural networks to detect outlier observations during prediction, inspired by principles widely used in chemometrics. By exploiting the transforms learnt by deep neural networks themselves, we can define provide a sense of distances within the network. This allows us to add prediction-time outlier detection to models after training without altering architecture or training. By drawing on the long experience of practical problem-solving in chemometrics, we contribute to safer use of deep learning.

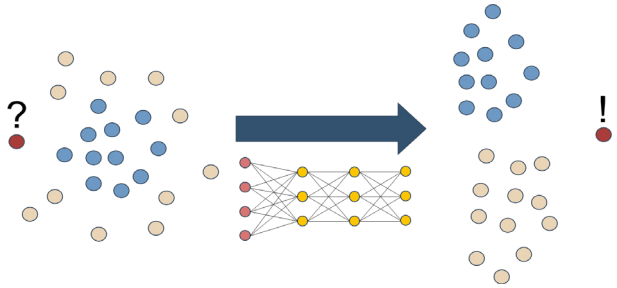

FIGURE 1. ILLUSTRATION OF OUTLIER DETECTION IN NEURAL NETWORKS.

P8

Influence of cook stove technology and fuels on particle emissions - A detailed characterization on physical and chemical properties

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Today air pollution is globally the leading environmental cause of disease and responsible for 9 million premature deaths annually. This burden has a disproportionately impact poor and vulnerable people living in remote areas in developing countries. The traditional practices used for cooking food leads to high exposures of particles with a diameter of less than one micrometre (PM1). Extensive efforts are being made on both improving the cook stoves and up-grading of biomass fuels to reduce the PM1 emissions. However, little is known about the characteristics of the particle emitted from these new stoves in combination with the new fuels, thus their impact on climate and health.

In this study PM1 emissions from four cook stoves with different technological advancements were compared; a 3-stone open fire, a rocket stove (both using wood sticks from two typically used tree spices; Sesbania and Casuarina), a natural draft gasifier stove, and a forced draft gasifier stove (both using pellets from soft wood and sugarcane bagasse). Emission performance was determined using a modified water boiling test where water (5L, 20°C) was brought to a boil and let simmer for 45 min, during which emissions were collected on filters. PM1 emission performance was determined by 1) total PM1 which was further fractionated into 2) inorganic elements, 3) organic carbon, and 4) elementary carbon.

Results show that the use of sesbania as fuel generated twice as high PM1 emissions as for using casuarina in both the 3-stone open fire (12.2 versus 6.2 $g/kg_{dry,fuel}$) and the rocket stove (6.2 versus 3.4 $g/kg_{dry,fuel}$). However, in the 3-stone open fire the main reduction was in the organic carbon fraction whereas in the rocket stove the inorganic fraction was mainly reduced. For the natural draft and force draft gasifier stoves the effects of fuel types were less pronounced, PM1 reduced from 2.2 to 1.4 $g/kg_{dry,fuel}$ and 0.3 to 0,2 $g/kg_{dry,fuel}$, in both cases the largest reduction was in the elementary carbon fraction.

We show that PM1 emission can be extensively reduced through a change to a more advanced cook stove, however PM1 emission are also high subject of change in amount and composition due to the fuel.

Information from Infrastructures

I9

The Biochemical Imaging Centre Umeå - BICU

The Biochemical Imaging Centre Umeå (BICU) provides state-of-the-art imaging technology including advanced light microscopy, affinity measurements and atomic force microscopy. BICU is an open-access imaging centre that offers cutting-edge techniques to researchers all over Sweden according to a fixed organization and user fees as described on the homepage. The centre includes dynamic live cell confocal microscopy and super-resolution microscopy. The state-of-the-art Atomic force microscopes allow for ultra resolution 3D-imaging and force-interaction measurements. Furthermore, the centre provides real-time quantification of binding of biosensors through solid-phase interaction techniques. Apart from providing microscopy services we also actively take part in programs aimed at training young researchers in the use of the basic as well as advanced microscopic techniques.

BICU is part of a **National Microscopy Infrastructure (NMI)**: a Swedish infrastructure for the use and support of advanced microscopy in life science. The mission of NMI is to provide faster access to innovative technology and competence in microscopy for the life science research community. NMI also coordinates national and international knowledge exchange in microscopy. NMI in Umeå is the node specialized for advanced correlative imaging techniques. Hereby, BICU closely collaborates with Umeå Core Facility for Electron Microscopy (UCEM) to provide correlative light and electron microscopy (CLEM).

EQUIPMENT

Zeiss ApoTome microscope (KBC building, H6)
Nikon A1R Laser Scanning Microscope (KBC building, H6)
Zeiss Spinning Disk Confocal Microscope (KBC building, H6)
Zeiss 710 Laser Scanning Microscope (6L, Oncology Department)
Bruker Atomic Force Microscope (KBC building, H6)
Biacore 3000 (KBC Building, A5)
Auto-ITC$_{200}$ (KBC Building, A5)
Proteon XPR36 (KBC Building, A5)
Ligand Tracer® Green (KBC Building, A6)

SERVICES

- Consultation, advice on experimental design and optimization of experimental conditions
- Technical support
- Personal training to provide drivers license for the user on the instrument
- Assistance with data analysis
- Data storage

CONTACTS

Facility Director: Richard Lundmark, richard.lundmark@umu.se
Facility Manager: Irene Martinez Carrasco, irene.martinez@umu.se
Senior Research Engineer for CLEM: Naga Venkata Gayathri Vegesna, gayathri.vegesna@umu.se

The biogeochemical analytical facility - BAF

The infrastructure provides instruments for analysis of key chemical parameters in terrestrial and aquatic biogeochemical and ecological research and as such is of major interest for a large range of research groups. BAF act as a core analytical facility for several major research projects run by researcher at EMG together with their collaborators and now opens up for other users at Umeå and other universities.

INSTRUMENTS

The facility covers a scope of different instruments including:

- Gas chromatograph (set up for analyses of CO^2, CH_4, C_3H_8, C_2H_4)
- TOC analyzer (also including particulate carbon)
- Nutrient analyzer (NO_3+NO_2, NH_4, PO_4, TN, TP) with possibilities to also analyze chloride
- Fluorometer
- Liquid scintillation counter (^3H, ^{14}C)
- Flow cytometer
- Respicond facility (to measure respiration)

CONTACTS

For analyses contact: Anders Jonsson
Department of Ecology and Environmental Sciences
Mobile: 070-2778659
E-mail: anders.jonsson@umu.se

I10

Biopolymer Analytical Platform - BAP

The Biopolymer Analytical Platform (BAP) is dedicated to support research among KBC groups on cell walls of terrestrial and aquatic plants, and biopolymer materials. Our competence lies in applying a large range of standard methods for the analysis of lignocellulose, as well as in fine detection of soluble sugars and starch. The methods include carbohydrate and lignin composition analysis using conventional wet chemistry and state-of-the-art analytical devices. The instrumental backbone for many of those methods is gas chromatography/mass spectrometry (GC/MS). Pyrolysis-GC/MS is one of the most important analytical tools that quickly yields highly reproducible and comprehensive chemical fingerprinting of carbohydrate and lignin types in samples in the lower microgram range.

Our service is open even for external research groups (outside KBC), however, there are different price categories for KBC and external groups. Postdocs, PhD students or project students with good lab work skills are required to do sample preparation in the BAP lab. We also provide an option to hire a professional staff hourly, in case your group has a lack of lab workers for sample preparation. It is possible to try a new method with us in the form of a project.

EXAMPLES FOR APPLICATIONS

- Pyrolysis-GC/MS for carbohydrate and lignin (G, S and H types) content estimation and for identification of organic compounds in soil/sediment
- TMS/Alditol acetate sugar-GC/MS for monosaccharide composition analysis
- Updegraff cellulose/anthrone assay for crystalline cellulose determination
- Klason, thioglycolic acid and acetylbromide lignin assay for lignin determination
- Enzymatic assays for soluble sugar (sucrose, glucose and fructose) and starch detection
- Size exclusion chromatography (SEC) for determination of MW, DP etc. of lignocellulose polymers

CONTACT INFORMATION

Webpage: https://www.upsc.se/resources/cell-wall-analysis.html
First contact for the customer: Laboratory manager, Junko Takahashi-Schmidt (Junko.TS@slu.se)

STEERING COMMITTEE

Totte Niittylä (Director), Dept. of Forest Genetics and Plant Physiology, SLU
Ewa Mellerowicz, Dept. of Forest Genetics and Plant Physiology, SLU
Hannele Tuominen, Dept. of Plant Physiology, UmU
Leif Jönsson, Dept. of Chemistry, UmU
Ola Sundman, Dept. of Chemistry, UmU
Junko Takahashi-Schmidt, Dept. of Forest Genetics and Plant Physiology, SLU

I12

Chemical Biology Consortium Sweden - CBCS

CBCS Umeå (former LCBU) is part of the national SciLifeLab infrastructure service in Chemical Biology. The objective of CBCS is to provide Swedish researchers help to identify and develop chemical research tools for their research. This is achieved through both updated research facilities/equipment and staff with expertise in assay development, small molecule screening, medicinal and computational chemistry and profiling of compound quality. In addition, we have state-of-the-art compound collections that can be used in screening projects to identify compounds that target the biological processes of interest to the individual researcher. This approach can be used for both basic and applied research in e.g. life sciences and plant research.

Resources provided by CBCS are made available through a peer-review-process. Projects are prioritized based on merit, scientific impact and practical feasibility. CBCS Umeå also has an instrument park that can be accessed through different collaborative forms or user agreements.

CBCS recently entered a research collaboration with AstraZeneca. This collaboration will provide access for Swedish academic researchers to AstraZeneca's annotated small molecule compound library consisting of roughly 14,000 compounds specifically targeting over 1,700 human proteins.

EQUIPMENT AT CBCS UMEÅ

- Plate readers, i.e. Biotek Synergy H4 with Biostacker and Tecan 200
- High Content Screening Microscope – Thermo Scientific Array Scan VTI
- Liquid handling robotics, Beckman Coulter NxP with 96- and 384-well head.
- HPLC, Gilson & Shimadzu

SERVICES PROVIDED

- Development of biological assays compatible with high-throughput screening
- Biochemical (target based) and cell-based high throughput screening
- High-throughput imaging technology
- Computational chemistry & modelling
- Medicinal chemistry expertise
- General expertise in preparative and analytical chemistry
- Assay development and screening with bacteria, viruses, and fungi (BSL-2)
- Theoretical and practical courses in High Throughput Screening

CONTACTS

Department of Chemistry, KBC-building, Floor 4C
Erik Chorell: erik.chorell@umu.se
Stina Berglund Fick: stina.berglund.fick@umu.se

MORE INFORMATION

www.cbcs.se
www.kbc.umu.se/english/lcbu/
www.scilifelab.se/facilities/cbcs

Technical platforms at Umeå Marine Sciences Centre

Chemical and biological analysis of marine samples

The platform provides analytical instruments and technical equipment for chemical and biological analysis of marine samples. The instruments are calibrated regularly, and the expert staff provides necessary training. Analysis of samples may be ordered from the accredited laboratory specialized in marine samples. The platform also offers research vessels and advanced sampling equipment for sampling in the marine environment. A long term marine environmental database is available for background data on chemical and biological parameters.

Mesocosm facilities

The indoor mesocosm facility includes 12 mesocosms with control of a large number of physical parameters, such as light, temperature, chemical composition of water, thermocline and rate of convective stirring. The facility has been upgraded so that projects that require ice covered water surfaces can be performed. The upgrade also includes state of the art lamps, and a ventilation that ensures natural levels of CO_2 in the room.

The outdoor mesocosm facility is not available at the moment since it is waiting for renovation.

Standardisation of sea/lake based mesocosms are performed at UMSC within the H2020 **Aquacosm** project.

EXAMPLES OF RESEARCH

• Lefebure, R et al. 2013. **Impacts of elevated terrestrial nutrient loads and temperature on pelagic foodweb efficiency and fish production**. Global Change Biology 19(5):1358-1372.
• Jonsson, S. et al. 2017. **Terrestrial discharges mediate trophic shifts and enhance methylmercury accumulation in estuarine biota.** Science Advances, 3(1)
• Båmstedt U., Larsson H. 2018. **An indoor pelagic mesocosm facility to simulate multiple water-column characteristics.** Int Aquat Res 10:13–29.
• Jonsson, S. et al. 2014. **Differentiated availability of geochemical mercury pools controls methylmercury levels in estuarine sediment and biota.** Nature Communications, 2014 Vol.5.
• Ripszam, M. et al. 2015. **Effects of predicted climatic changes on distribution of organic contaminants in brackish water mesocosms**. Science of the Total Environment 517: 10-21.
• Wikner, J., Andersson, A. 2012. **Increased freshwater discharge shifts the trophic balance in the coastal zone of the northern Baltic Sea.** Global Change Biology, 18(8): 2509-2519.

TEACHING ACTIVITIES / COURSES

Mainly PhD courses, for example NMA-course **Can eutrophication in the Baltic Sea be counteracted?**

CONTACT

Umeå Marine Sciences Centre, Norrbyn, Hörnefors
Siv Huseby, Environmental analyst, siv.huseby@umu.se
Henrik Larsson, Senior research engineer, Henrik.larsson@umu.se

I15

NanoLab

NanoLab is a classified Class 100 cleanroom located at the department of Physics. It was established in June 2012, and has since its inception been in continuous development. Today, it comprises a variety of advanced fabrication and characterization setups, including, **thin-film deposition system (PVD75 thermal evaporator), nanoimprinter (Obducat NIL 2.5), mask aligner (Karl Süss Mask Aligner MJB3, X-ray diffractometer (PANalytical Xpert3 Powder), optical tensiometer (Attension Theta), low-pressure plasma system (diener electronics ATTO)**, as well as number of more standard pieces of equipment, such as spin coaters, optical microscopes, vacuum ovens, hotplates, UV-curing boxes, analytical scales, etc.

Besides the equipment available in the Nanolab, the Nanolab offers space for user´s own experiment too. Users have access to fume hoods and central gases (N_2, Ar, H_2, O_2, liquid CO_2, compressed air) and vacuum in each working station and inside the fume hoods.

Manuals for all equipment are to be found in this website, shorter version manuals are available too in the NanoLab.

Trainings are offed annually for using the cleanroom and for the most of the equipment. Check KBC website for recent course announcements or contact Dr. Roushdey Salh (the coordinator of the NanoLab).

The equipment in NanoLab is made available to all scientists at Umeå University, as well as external institutions, for just a minor fee. A discount is offered for frequent users or high-volume users.

The infrastructure is supported by KBC and supervised by experts from department of Physics, Microbiology, and Applied physics and electronics. The NanoLab is used for both research and to educate student in advanced levels.

The NanoLab has special environment, with this unique opportunity comes many responsibilities and restrictions. All users are kindly asked follow the general rules of a cleanroom and to keep an active eye on the overall facilities and taking part in improving the cleanroom. Therefore every user must take part in the cleanroom training seminar before having the license to use the NanoLab and the facilities independently.

The most important cleanroom rules:

- Only trained users can enter the cleanroom.
- Follow the special entrance and exit procedures.
- No pencils, papers, rings, watches, mobile phones are allowed in the cleanroom.
- No cosmetics when intending to use the cleanroom.
- No smoking 30 minutes prior to entering the cleanroom.
- Prevent touching any objects or surfaces unnecessarily.
- Prevent fast moving or talking in the cleanroom.
- Clean after finishing your work.

CONTACT INFORMATION

Roushdey Salh, roushdey.salh@physics.umu.se

I17

Protein Expertise Platform - PEP

The Protein Expertise Platform (PEP) is a strong environment at the Chemical Biological Center (KBC), at Umeå University. The PEP provides researchers with needed services and expert advice in questions of bioinformatics, cloning, growth optimization and protein purification. The PEP keeps stocks of over 20 different ready to use cloning vectors (containing a variety of fusion proteins and purification tags) designed to improve protein expression levels and to facilitate protein purification. In addition, the PEP provides about 10 different strains of competent *E.coli* bacteria ready for transformation, as well as various antibiotics and different proteases that are commonly used in protein purification.

MATERIAL

The PEP provides researchers with the necessary materials for cloning and protein expression, having in stock a variety of cloning plasmids, antibiotics and competent bacteria cells. Further, commonly used proteases for tag removal by site specific cleavage can be obtained. We can also provide you with material for isotopic labeling.

CLONING

We can help you with your cloning issues e.g. PCR, ligation, subcloning, and mutagenesis.

PROTEIN EXPRESSION SCREEN (SMALL SCALE)

We can set up a small scale screening in order to see if your protein of interest is expressed and soluble. If you experience problems with protein expression due to low solubility or low expression, we can set up a small scale experiment to test a number of different fusion partners and bacterial host cells.

PROTEIN EXPRESSION AND PURIFICATION (SCALE UP)

If you need a larger amount of your protein or if you have problems with low expression levels, we can scale up the culture used for protein production. We also offer protein purification using Affinity tags, IEX and SEC.

EDUCATIONAL ACTIVITIES

Graduate courses such as the fast "Cloning, Protein Expression and Purification" (CPEP), "Protein Crystallization" and "Basic Bioinformatics" courses address many topics of high interest for young researchers. Taking our courses enables them to independently solve general problems ranging from sequence analysis, primer design, molecular cloning to protein construct design and purification.

CONTACT

Mikael Lindberg, PhD, Senior research engineer
Dept of Chemistry, Umeå University, 901 87 Umeå. E-mail: mikael.lindberg@umu.se

I18

The Proteomics Core Facility at KBC

The proteomics facility was initiated in 2003 and became in 2009 a part of the KBC research infrastructure. It provides infrastructure and services for research in protein science and mass spectrometry-based proteomics, and it has the homepage: www.kbc.umu.se/english/proteomics. The equipment of the facility includes two electrospray mass spectrometers for LC-MS applications and bioinformatics resources for on-line booking of instruments, data storage and an in-house Mascot server, which provides access to many important sequence databases. The facility also developed solutions for long-term storage and archiving of large scale proteomics dataset, which meet the demands of arching of research data Swedish universities.

The analytical applications provided include mass determinations of proteins and peptides by ESI- MS, protein identifications using ESI-LC-MS/MS, qualitative and semi-quantitative expression proteomics, and analysis of post-translational modifications such as phosphorylation. In their teaching work, the staff of the facility have offered courses for the graduate schools at KBC and UCMR and contribute to the teaching the Department of Chemistry and the Umeå Plant Science Center. In addition, the teaching activities also included organization of other events within the KBC such as the KBC Mass Spectrometry Day, the first Scandinavian Plant Proteomics Day and bioinformatics workshops in collaboration with SciLifeLab at the BMC Uppsala.

CONTACT INFORMATION

The current facility members are Professor Gunnar Wingsle and Dr. Thomas Kieselbach. Contact: Gunnar Wingsle, Department of Forest Genetics and Plant Physiology of the Swedish University of Agricultural Sciences, gunnar.wingsle@slu.se. Thomas Kieselbach, Department of Chemistry of Umeå University, thomas.kieselbach@umu.se.

Recent research projects that were supported by the facility include:

• Zhang X, Dominguez PG, Kumar M, Bygdell J, Miroshnichenko S, Sundberg B, Wingsle G, Niittylä T (2018). Cellulose synthase stoichiometry in Aspen differs from *Arabidopsis* and Norway spruce. Plant Physiol. 177: 1096-1107. doi:10.1104/pp.18.00394.

• Kieselbach T, Cheregi O, Green BR, Funk C (2018). Proteomic analysis of the phycobiliprotein antenna of the cryptophyte alga *Guillardia theta* cultured under different light intensities. Photosynth Res. 135: 149-163. doi:10.1007/s11120-017-0400-0.

• Bygdell J, Srivastava V, Obudulu O, Srivastava MK, Nilsson R, Sundberg B, Trygg J, Mellerowicz EJ, Wingsle G (2017). Protein expression in tension wood formation monitored at high tissue resolution in *Populus*. J Exp Bot. 68: 3405-3417. doi: 10.1093/jxb/erx186.

• Obudulu O, Bygdell J, Sundberg B, Moritz T, Hvidsten TR, Trygg J, Wingsle G. (2016) Quantitative proteomics reveals protein profiles underlying major transitions in aspen wood development. BMC Genomics. 17: 119. doi: 10.1186/s12864-016-2458-z.

• Espaillat A, Forsmo O, El Biari K, Björk R, Lemaitre B, Trygg J, Cañada FJ, de Pedro MA, Cava F. (2016) Chemometric analysis of bacterial peptidoglycan reveals atypical modifications that empower the cell wall against predatory enzymes and fly innate immunity. J Am Chem Soc 138: 9193-9204. doi: 10.1021/jacs.6b04430.

I19

Swedish Metabolomics Centre - SMC

Swedish Metabolomics Centre (SMC; www.swedishmetabolomicscentre.se) was launched 2013 via an infrastructure grant from Knut & Alice Wallenberg Foundation and co-funding from Umeå University, Swedish University of Agricultural Sciences and Chalmers Technical University. From 2016 SMC is a part of SciLifeLab. The main aim of the centre is to support the researchers at Swedish Universities with mass spectrometry based small molecule, lipid and metabolomics analysis in biological tissues and fluids, and furthermore, to become a leading knowledge centre in metabolomics and related areas.

SERVICES

All service request starts with a meeting between the SMC and the customer, either in person or over the phone or Skype, to better understand the customer's research question and together decide the analysis of choice. SMC also offers an Open lab access service (OAP-service), where researchers after training by SMC personnel can rent an instrument and perform analysis themselves.

- Untargeted metabolite profiling (metabolomics)
- Targeted metabolite profiling, e.g. amino acids, sugars, fatty acids, TMAO (for details, contact Head of Facility).
- Targeted lipid profiling (for details, contact Head of Facility).
- Study design
- Method development
- Basic statistics
- Open lab access services

EQUIPMENT

Mass spectrometers

- Leco Pegasus BT, GCTOFMS
- Leco Pegasus HT, GCTOFMS
- Agilent 7000C, GCQqQMSMS
- Thermo Scientific LTQ-Orbitrap XL
- Agilent UHPLC-QqQMSMS 6495
- Agilent UHPLC-QqQMSMS, 6490 (2)
- Agilent 6550 iFunnel Accurate-Mass UHPLC-QTOFMSMS (2)
- Agilent 6560 Ion Mobility UHPLC-QTOFMSMS

CONTACT

For service requests or questions please contact: info@swedishmetabolomicscentre.se

Facility Director: Prof. Thomas Moritz (thomas.moritz@slu.se), +46 90 786 8456
Deputy Facility Director: Ass. Prof. Anders Nordström (anders.nordstrom@umu.se), +46 90 785 2561

Head of Facility: Dr. Annika Johansson (annika.johansson01@umu.se), +46722445254

I20

The Trace Analysis Platform – TAP

A Technical Platform at the Department of Chemistry

This platform aims to provide state-of-the-art equipment, user training and support for trace analysis of small molecules in complex matrices, such as environmental and biological samples.

The platform supports the detection of minute quantities of analytes such as metals, organic compounds, and organometallic compounds with both qualitative and quantitative methods. For metals and organometallic compounds both total concentrations and speciation is supported.

APPLICATION EXAMPLES

The equipment that forms the foundation of the platform is or has been supporting work in the following areas:

- Trace element analysis (metals, phosphorus, sulphur, chlorine and bromine)
- Speciation (Hg, Sn and As compounds)
- Protein-metal complexes and interactions
- Trace analysis of persistent organic pollutants (POPs)
- Multi-residue analysis of pharmaceuticals
- Indoor air pollutant and metabolomics studies
- Non-target screening/characterization and identification of unknowns

INSTRUMENTATION

The platform has mass spectrometry based equipment, most often coupled to initial chromatographic separation, encompassing the following fields:

- Organic GC-MS
- Organic LC-MS
- Organo-Metal ICP
- Isotope-ratio and direct liquid inlet MS

SERVICES

The platform primarily provides access to instrumentation, but can also provide analytical services and operator training. The services may include: design of experiments, sample preparation, instrumental analysis and interpretation of data. Service is provided at three different levels:

- Seed projects (a few samples)
- Small projects (10s of samples)
- Projects and long-term service (100s of samples)

Contact the relevant co-ordinator for questions on availability, prices and level of support.

CONTACT INFORMATION

The facility is located on the 6:th floor in the KBC building.

Main Contact:	Peter Haglund	Director, 090-786 6667
Co-ordinators:	Erik Björn	ICP-MS, 090-786 5198
	Peter Haglund	Non-Target MS Analysis, 090-786 6667
	Per Liljelind	GC-MS, 090-786 9321
	Richard Lindberg	LC-MS, 090-786 5464

Webpage: http://tap.chem.umu.se/

Umeå Core Facility for Electron Microscopy – UCEM

UCEM provides instruments and methods in Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) as a national research infrastructure. UCEM is an interdisciplinary core facility for imaging and advanced Electron Microscopy (EM). UCEM houses six EM instruments, sample preparation equipment as well as computer infrastructure and software for image processing. The facility staff provides service and training to users in the user-friendly EM labs, where students and scientists can perform advanced sample preparation, imaging and image analyzes.

The Zeiss SEMs, Merlin and Evo, offer high-resolution surface imaging, with multiple detector systems operating under cryo, room temperature or heated conditions. Correlative Light and Electron Microscopy (CLEM) solutions for finding the precise location of a target proteins or structure of interest simplifying localization and high-resolution imaging of the same sample. The FEI Scios DualBeam is an unique instrument in Umeå, combining SEM with a Focused Ion Beam (FIB) for micro-manipulation, volume imaging through Slice & View methodology and thin lamella preparation for subsequent TEM analyses.

The TEM instruments Jeol 1230 and FEI Talos L120 offer ideal TEM solutions for entry level and sample screening, electron tomography and CLEM. Service at UCEM also includes cell and tissue fixation, resin embedding, ultra-microtome sectioning, Tokuyasu sectioning, immunolabeling and staining techniques. Cryo-EM is the method of choice for visualization of hydrated proteins, viruses, cells and small organisms. Samples are plunge frozen in liquid ethane, preserved in amorphous ice and imaged under cryo-condition with FEI Titan Krios 300 kV, equipped with autoloader for cryo samples, a phase plate for contrast enhancement and two direct electron detectors, Falcon3 and K2 BioQuantum. Single particle reconstruction is used for structure biology and cryo-electron tomography is used to study e.g. membrane complexes and subcellular volumes in 3D.

Together with the Biochemical Imaging Centre Umeå (BICU), UCEM provides CLEM imaging support as part of the National Microscopy Infrastructure (NMI). The cryo-EM facility is a SciLifeLab node and part of CryoNet, a Swedish-Danish partnership. The establishment of an advanced EM facility in Umeå was made possible through funding by the Swedish Research Council, Knut and Alice Wallenberg Foundation and the Kempe Foundations.

CONTACT

For general enquiries:

Linda Sandblad, Facility Coordinator / Head of Facility

Visiting address: Electron Microscopy Building (former Säkerhetshuset), KB-D, Umeå University

Mobile: +46 (0)70 932 49 36, E-mail: linda.sandblad@umu.se

http://www.kbc.umu.se/english/ucem/

I24

Vibrational Spectroscopy Core Facility - ViSp

ViSp provides FT-IR and Raman spectroscopy and microspectroscopy services, ranging from design of experiments to measurements and data analysis. ViSp has state-of-the-art instrumentation, including vacuum bench FTIR spectrometers, FTIR microscopes with focal plane array detectors, a confocal Raman microscope with 5 laser lines, a fiber optic probe and polarizers, and a portable Raman spectrometer. The techniques are suitable to detect (and localise at micron and submicron level) chemical changes in a wide range of samples, at high speed and low cost, non-destructively and label-free. ViSp can provide both hardware and software development to adapt the techniques to the needs of the users / projects.

EXAMPLE APPLICATIONS/RESEARCH PROJECTS

Due to the exceptional versatility of the techniques, example projects covers a wide range of scientific disciplines and applications. Among the most prominent are materials sciences (nanotechnology, semiconductors), plant sciences (high-throughput chemotyping/screening, investigating the effects of gene manipulations or environmental factors), chemistry (absorption on mineral surfaces, real-time, in situ monitoring of reactions, protein conformational changes) and medicine (assessing tissue compositional changes under various pathological conditions, diagnosing and monitoring disease onset and progression, drug targeting and molecular mechanistic studies). ViSp is primarily research driven and actively participates in projects where new methods need to be developed as well as applying existing methodologies in new areas.

TEACHING ACTIVITIES / COURSES

A User License Course is run twice a year, giving a basic introduction to vibrational spectroscopy in general and training users in running their own experiments at ViSp. ViSp is also involved at numerous courses at Umeå University and SLU.

LOCATION

Chemistry Department, Building C, floor 1 (microspectroscopy) and floor 6 (spectroscopy).

CONTACT

András Gorzsás, manager
andras.gorzsas@umu.se
http://www.kbc.umu.se/english/visp/

I25

The X-ray Crystallography Platform

The X-ray Crystallography Platform provides crystallographic expertise and access to state of the art equipment for crystal set-ups and data collection. Single crystal X-Ray Diffraction (XRD) provides 3D structural information at atomic resolution of small molecules as well as macro-molecules such as proteins, DNA, RNA, and their complexes. XRD is ideally suited for drug target screening ("High Throughput Screening") and "Fragment Based Drug Discovery" by determining the structure of proteins with bound drug candidates. In addition, the X-ray equipment can be used for powder and fibre diffraction.

EQUIPMENT

- Nano-drop crystallization robot (mosquito®, TPP LabTech) for screening of crystallization conditions
- A Formulatrix "Rockimager" crystallization imaging and storage cabinet and a "Rockmaker" liquid handling robot
- A high brilliance X-ray diffraction system (X8 PROTEUM, Bruker AXS) that produces a fine focused, monochromatic X-ray beam of a wavelength $\lambda = 1.54$ Å (Cu-Kα radiation). Crystals are positioned in the beam with a kappa goniometer
- A CryoStream 700 (Oxford) maintains the crystals at 100K during data collection
- High-end computing equipment and sophisticated software for data collection and analysis
- The platform has direct access to an Agilent 1200 Series High-Throughput LC/UV/Mass-Spec system

SERVICE

- Screening of crystallization conditions using the nano-drop pipetting robot (mosquito®)
- Monitoring, evaluation and scoring of crystallization screens
- Optimization of initial screens
- Diffractions tests and iterative crystal optimization (diffraction quality and resolution)
- Full diffraction data collection incl. data processing and data analysis
- X-ray crystal structure determination, refinement and validation
- Deposition of coordinates with the Protein Data Bank (PDB) or the Cambridge Structural Database (CSD)
- Compound screens: co-crystallization with fragments and compounds (in collaboration with LCBU)
- Cryogenic preservation of crystals (vitrification) and storage in liquid nitrogen
- Powder data collection

CONTACT

Uwe Sauer (coordinator): tel: 090-786 5930 e-mail: uwe.sauer@umu.se
http://www.kbc.umu.se/english/x-ray/

X-ray photoelectron spectroscopy platform - XPS

The X-ray photoelectron spectroscopy (XPS) platform is an open infrastructure at Umeå University enabling users both within UmU and outside to obtain analyses of the chemical composition of their sample surface. Knowledge of the elemental composition, oxidation state and spatial distribution of atoms at surfaces, near-surfaces, and interfaces is crucial to our understanding of key reactions in nature and technology. Surfaces are, after all, the interface through which materials - as small as nanoparticles and bacteria, to as big as nuclear fuel reactors and spaceships - interact with their environments. XPS, also known as Electron Spectroscopy for Chemical Analysis (ESCA), is now one of the most widely used tools in countless fields of science and engineering where advanced analyses of surfaces and interfaces is needed.

The platform provides surface analysis by XPS technique. Full range of conventional XPS experiments is available including monochromatic Al Kα excitation, angle-resolved XPS, XPS imaging, and cryogenic measurements.

EQUIPMENT

AXIS Ultra DLD is an electron spectrometer manufactured by Kratos Analytical, Ltd. (UK). The instrument was installed at the Dept of Chemistry in 1999 and upgraded twice with a Delay-Line-Detector in 2004 and new X-Ray power supply in 2009.

SERVICE

In the outermost 10 nm of a surface (10 atomic layers), XPS provides:

- Identification of all elements (exc. H and He) present in concentrations >0.1 atomic %
- Semi quantitative determination of the elemental surface composition
- Information about the molecular environment (oxidation state, bonding atoms, etc.)
- Non-destructive elemental depth profile 10 nm into the sample and surface heterogeneity assessment
- Lateral variations in surface chemical composition (XPS imaging with spatial resolution of 5 µm)
- Studies on wet/hydrated (frozen) samples

The XPS platform is **the only facility for XPS analyses in Northern Sweden** (north of Uppsala). The platform supports a unique field of research, developed at the Department of Chemistry involving investigations of fast-frozen samples including mineral-aqueous solution interfaces, interfaces of biomaterials with biologically relevant media, and surface chemistry of microorganisms. The platform also supports a large range of research areas by providing state-of-the-art surface analysis in areas including ecology, chemistry, physics, archeology, molecular biology and engineering.

STEERING BOARD

Andrey Shchukarev (Researcher, Dept of Chemistry), Knut Irgum (Prof., Dept of Chemistry), Madeleine Ramstedt (Lecturer, Dept of Chemistry), Jean-François Boily (Prof., Dept of Chemistry)

CONTACT INFORMATION

Andrey Shchukarev, Dept of Chemistry, KB.C6, B6-35-07 (XPS lab) and B6-33-07 (office), tel. 090-786 5361.
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http://www.chemistry.umu.se/english/research/infrastructure/xps-spectroscopy/

I26

The Fluorescence In Situ Hybridization (FISH) facility

for environmental, clinical, food and biotechnology research

The goal of the Fluorescence In Situ Hybridization (FISH) research facility is to apply and develop novel cultivation-independent procedures to identify genes in intact whole cells or viruses in their natural environment based on phylogenetic markers. FISH can therefore complement not only other microscope based studies (e.g. fluorescence microscopy, electron microscopy) based on non-phylogenetic stains, but also disruptive molecular biological methods, which rely on the extraction of cellular components such as DNA. Thus, FISH can retrieve the information that is lost when extracting DNA for gene sequencing, for example morphology, distribution, single cell activity and association with other cells or viruses. FISH can be employed in different samples (environmental, clinical, food, industry/biotechnology), and can target all cell types (Archaea, Bacteria, Eukarya) and at least certain viruses. The most common gene target for cell identification is the ribosomal gene, but also housekeeping genes, functional genes, pathological genes, or even whole genomes can be targeted. FISH can be combined with other analytical methods, such as radioactive/isotope methods, flow cytometry, RAMAN spectroscopy, mass spectrometry, spectral imaging.

The KBC FISH research facility is located at the department of medical biochemistry and biophysics, and is managed by the department of ecology and environmental science. The research facility is equipped with all equipment necessary for FISH, including a large collection of gene probes for various taxa, reference samples, and a high performance computer for bioinformatics with a gene sequence database for phylogenetic studies, gene probe evaluation and design. Today, FISH is included in different research projects, e.g. in plant, fungal and animal biology, microbial geoecology, pathogen detection, and different industrial applications, e.g. wastewater treatment, cellulose-paper industry, and food production. In 2019, an interdisciplinary FISH course will be organized at KBC Umeå with different FISH experts within and outside UmU, for both students and researchers.

CONTACT

Natuschka Lee, Lab Microbial Geoecology and Astrobiology, Department of Ecology and Environmental Science and Department of Medical Biochemistry and Biophysics Chemical Biological Center (KBC), Umeå University. E-mail: natuschka.lee@umu.se

References:

• Lee NM. 2018. Whole Cell Identification of Microorganisms in their Natural Environment with FISH. Analytical Geomicrobiology. Cambridge University Press. Eds: D Alessi, H Veeramani, J Kenney. In press

• Borecki G, Lee NM. 2016. Rapid Microscope Based Identification Method for Tuberculosis and Other Mycobacteria: FISH. Tuberculosis. SMGebooks, USA

Overview Infrastructure Presentations

Scientific Infrastructure	Contact persons	Tour	Poster/code
Biochemical Imaging Centre Umeå (BICU)	richard.lundmark@umu.se Irene.martinez@umu.se	yes	**I9**
Biogeochemical Analytical Facility (BAF)	ann-kristin.bergstrom@umu.se anders.jonsson@umu.se	yes	
Biopolimer Analytical Platform (BAP)	totte.niittyla@slu.se junko.TS@slu.se		**I10**
Computational Life Science Cluster (CLiC)	johan.trygg@umu.se Jeanette.tangrot@umu.se joakim.bygdell@umu.se		**I11**
Chemical Biology Consortium Sweden (CBCS)	stina.berglund.fick@umu.se	yes	**I12**
Technical platforms at Umeå Marine Sciences Centre	siv.huseby@umu.se henrik.larsson@umu.se		**I13, I14**
NanoLab	roushdey.salh@umu.se		**I15**
Nuclear Magnetic Resonance Core Facility (NMR)	jurgen.schleucher@umu.se gerhard.grobner@umu.se	yes	**I16**
Protein Expertise Platform (PEP)	mikael.lindberg@umu.se uwe.sauer@umu.se	yes	**I17**
Proteomics Core Facility	gunnar.wingsle@slu.se thomas.kieselbach@umu.se	yes	**I18**
Swedish Metabolomics Centre (SMC)	annika.johansson01@umu.se	yes	**I19**
Trace Analysis Platform (TAP)	peter.haglund@umu.se	yes	**I20**
Umeå Core Facility for Electron Microscopy (UCEM)	linda.sandblad@umu.se	yes	**I21, I22, I23**
Vibrational Spectroscopy Core Facility (ViSp)	andras.gorzsas@umu.se	yes	**I24**
X-Ray Crystallization Platform (X-ray)	uwe.sauer@umu.se	yes	**I25**
X-Ray Photoelectron Spectroscopy (XPS)	andrey.shchukarev@umu.se	yes	
The Fluorescence In Situ Hybridization facility (FISH)	natuschka.lee@umu.se		**I26**

Coordinated services at KBC	Contact person/contact address
Mechanics workshop at the Department of Physics	peter.wikstrom@umu.se isak.silander@umu.se
KBC Communication office	Anna Shevtsova, Anne Honsel, info.kbc@umu.se
KBC Focus environment	Hardy Hall, hardy.hall@umu.se
KBC Service centre	servicecenter.kbc@umu.se
KBC Printing service	lars.aberg@umu.se
KBC IT-support (CAS Login)	http://kbc-support.ad.umu.se/IT/
KBC Chemical Store (CAS login)	https://chemshop.chem.umu.se

Participants

Last name	First name	E-mail	Affiliation
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