



Chemical Biological Centre Umeå University/SLU www.umu.se/en/kbc



# **KBC DAYS 2019** 5-6 November, KBC-building

### Programme - Abstracts - Research Infrastructures



### 8.30 Registration and poster mounting

#### SESSION 1

Chairperson: Stefan Björklund

#### 9.00 Welcome

Stefan Björklund Scientific Coordinator for KBC

#### 9.10 Closer research infrastructure collaboration between SLU and UmU? Göran Ståhl

Dean, Faculty of Forest Sciences, SLU

## 9.25 Connecting DNA replication stress to checkpoint initiation

Peter Burgers

Washington University School of Medicine, St. Louis, Missouri, United States. Visiting Professor at the Department of Medical Biochemistry and Biophysics, Umeå University

### 10.10 Coffee break

### **SESSION 2: LIFE SCIENCE IN UMEÅ**

Chairperson: Sylvia Larsson

- 10.40 Inflammasomes and Reactive Oxygen Species Saskia Erttmann Department of Molecular Biology, Umeå University
- 10.55 Predicting mutational routes to new adaptive phenotypes Peter Lind

Department of Molecular Biology, Umeå University

#### 11.10 Pressures and flows in the brain Anders Eklund Department of Radiation Sciences, Umeå University

11.25 The SLU Stable Isotope Laboratory – how can isotopes improve your research? Mats Öguist

Department of Forest Ecology and Management, SLU

- 11.40 Regulation of gene expression by RNA mods Francesca Aguilo Department of Medical Biosciences and Wallenberg Centre for Molecular Medicine at Umeå University (WCMM), Umeå University
- 11.55 Lunch

## SESSION 3: NEW FACULTY MEMBERS, AWARD AND GRANT RECIPIENTS AT KBC

Chairperson: Paulina Wanrooij

#### 13.15 The large KAW projects at UPSC Ove Nilsson Umeå Plant Science Centre (UPSC), Department of Forest Genetics and Plant Physiology, SLU

### 13.35 Kempe Funded Postdoc Program in Integrated Structural Biology

Magnus Wolf-Watz

Department of Chemistry, Umeå University

#### 13.55 The replicative lifestyle of mobile elements in methicillin resistant *Staphylococcus aureus* Ignacio Mir-Sanchis

Department of Medical Biochemistry and Biophysics and Wallenberg Centre for Molecular Medicine at Umeå University (WCMM), Umeå University

14.15 Coffee break

#### SESSION 4: NEW FACULTY MEMBERS, AWARD AND GRANT RECIPIENTS AT KBC AND PRESENTATIONS FROM MIDTERM PHD STUDENTS

Chairperson: Ann-Kristin Bergström

### 14.50 AI lab for Life Science?

Johan Trygg

Department of Chemistry, Computational Life Science Cluster (CLiC), Umeå University

### 15.10 Getting to the Root of plant biology

Karin Ljung

Umeå Plant Science Centre (UPSC), Department of Forest Genetics and Plant Physiology, SLU

## 15.30 Coastal phytoplankton characterization for assessing ecological state

#### Agneta Andersson

Department of Ecology and Environmental Sciences (EMG), Umeå University

## 15.50 Efforts to support the development of the individual science career

Marianne Sommarin

Umeå Plant Science Centre (UPSC), Department of Plant Physiology, Umeå University

#### 16.10 PRESENTATIONS FROM MIDTERM PHD STUDENTS (2 minutes each)

#### Molecularly imprinted polymers in capillary monolithic format Chau Huvnh

Department of Chemistry, Umeå University

#### Using Life Cycle thinking to interpret sustainable performance of essential municipal services of cities. Wastewater and Municipal Solid Waste

Kavitha Shanmugam Department of Chemistry, Umeå University

### Mesoporous melamine-formaldehyde. A potential solution for utilization of CO<sub>2</sub>? Thai Q. Bui

Department of Chemistry, Umeå University

#### Strong effect of ageing on swelling properties of graphene oxide membranes in alcohols Artem Iakunkov

Department of Physics, Umeå University

### Hydrothermal pretreatment of sugarcane bagasse with and without sulfuric acid - New insights on effects of pretreatment severity

Dimitrios Ilanidis Department of Chemistry, Umeå University

## **CELLULOSE SYNTHASE INTERACTING 1** is required for wood morphogenesis and mechanics in aspen

Anne Bünder Umeå Plant Science Centre, Department of Forest Genetics and Plant Physiology, SLU

## Generation of A Mucin Glycopeptide Microarray Library for Evaluation of Host-Pathogen Interactions

Sandra Behren Department of Chemistry, Umeå University

### Implementation of machine learning for more comprehensive process understanding in wastewater treatment plant

Dong Wang Department of Chemistry, Umeå University

#### **Marine microorganisms for bioplastic production** Piotr Jablonski Department of Chemistry, Umeå University

#### Morphological Analysis of Apolipoprotein E Binding to Aβ Amyloid Using a Combination of Surface Plasmon Resonance, Immunogold Labeling and Scanning Electron Microscopy

Tohidul Islam Department of Medical Biochemistry and Biophysics, Umeå University

#### Fungal community responses to clear-cutting and addition of nitrogen to seedlings David Castro

Umeå Plant Science Centre, Department of Forest Genetics and Plant Physiology, SLU

## Activated graphene as electrode material in supercapacitors

Andreas Nordenström Department of Physics, Umeå University

16.35 Smoothies and fruits

### 16.40 POSTER SESSION

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

18.00 Dinner

### DAY 2, Wednesday 6 November

### **SESSION 5**

Chairperson: Fredrik Almqvist

### 9.00 Insect Biotechnology

Andreas Vilcinskas

Department of Insect Biotechnology, Justus-Liebig-University Giessen, Germany

### 9.45 Mechanics and dynamics of cell-to-cell adhesion in plants

Stéphane Verger

Umeå Plant Science Centre (UPSC), Department of Forest Genetics and Plant Physiology, SLU

#### 10.05 Control of plant development via temperaturedependent mRNA splicing Markus Schmid

Umeå Plant Science Centre (UPSC), Department of Plant Physiology, Umeå University

### 10.25 Coffee and presentation of the KBC Poster Award 2019

### **SESSION 6: LIFE SCIENCE IN UMEÅ**

Chairperson: Lena Gunhaga

#### **10.55** Type I interferons shape viral tropism in the brain Anna Överby Wernstedt

Department of Clinical Microbiology and Molecular Infection Medicine Sweden (MIMS), Umeå University

## 11.10 Targeting tumor-stromal interactions in pancreatic cancer

Daniel Öhlund

Department of Radiation Sciences and Wallenberg Centre for Molecular Medicine at Umeå University (WCMM), Umeå University

# 11.25 Understanding the mechanisms modulating the interactions between herpes simplex virus and cell-surface glycosaminoglycans

Marta Bally

Department of Clinical Microbiology and Wallenberg Centre for Molecular Medicine(WCMM), Umeå University

## **11.40** Into thin air: how to sense and adapt to low oxygen Changchun Chen

Umeå Centre for Molecular Medicine (UCMM) and Wallenberg Centre for Molecular Medicine (WCMM), Umeå University

### 11.55 Transforming growth factor beta and oncogenic signaling pathways in prostate cancer Maréne Landström

Department of Medical Biosciences, Umeå University

### DAY 2, Wednesday 6 November

### 12.30 Lunch

### **SESSION 7**

Chairperson: Florian Schmidt

### 13.10 Umeå University's innovation system Karin Borge Renberg Umeå University Innovation Office and Umeå universitet holding AB

## **13.15** Regulatory CTPases as central players in bacterial chromosome segregation

Martin Thanbichler

Faculty of Biology at Philipps University, Max Planck Institute for Terrestrial Microbiology, and the LOEWE Center for Synthetic Microbiology (Synmikro), Marburg, Germany

#### 14.00 Centre for Sustainable Cement and Quicklime Production at Umeå University Matias Eriksson

Department of Applied Physics and Electronics, Umeå University, and Centre for Sustainable Cement and Quicklime Production

## 14.20 Curious about science? Communicating science through hands-on activities

Madelen Bodin

Department of Science and Mathematics Education, and Director of Curiosum, Umeå University

#### 14.35 PANEL SHOWCASE DISCUSSION BY THE KBC INFRASTRUCTURES

**15.05** Coffee and

### GUIDED TOURS ORGANISED BY THE KBC INFRASTRUCTURES

(Sign up for the tours at the registration desk)

- Biochemical Imaging Centre Umeå, BICU
- Chemical Biology Consortium Sweden, CBCS Umeå
- NMR Core Facility
- Swedish Metabolomics Centre Umeå
- Umeå Core Facility for Electron Microscopy, UCEM
- Vibrational Spectroscopy Core Facility, ViSp
- Technical platforms at Umeå Marine Sciences Centre, UMSC (sign up at the registration desk. If enough people express their interest, a guided tour will be arranged later)

P-1

### Molecularly Imprinted Polymersin Capillary Monolithic Format

Chau Huynh, Mingquan Liu, Knut Irgum

Umeå University, Department of Chemistry, S-901 87 Umeå, Sweden

The research of our group focuses on synthesis of molecularly imprinted monoliths and surface grafting in both "conventional" synthesis based on vinylic monomers and our novel partly aqueous biphasic step-growth polymerization. These materials have been synthesized in situ in capillary format which inner diameter from 100 um to 250 um. Our most recent results address a key question in molecularly imprinted materials research: *"Which are the main epitopes responsible for recognition in surface imprinted materials?"* where tryptic fragments of ProGRP and phosphorylated peptides are used as example models.

This work has been performed as part of BioCapture project: "Smart capture phases for proteomics, glycomics and biomarker assays". This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No. 722171.

References

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### P-2

### Using Life Cycle thinking to interpret sustainable performance of essential municipal services of cities. Wastewater and Municipal Solid Waste

Kavitha Shanmugam, Mats Tysklind, Venkata K K Upadhyayula

Department of Chemistry, Umeå University, Umeå, Sweden

The ramifications of improving human lifestyle without considering environmental expenses can be quite complex. To strike a balance, the society have to be selfsustaining which essentially translates to an important objective of building cities that are immune to environmental pressures while simultaneously maximizing the social welfare of people. Sustainable city centric techno-entrepreneurial concepts, e.g. development of low cost and modular technologies for removal of micropollutants from treated wastewater, conversion of MSW to biofuels, recover phosphorus from sewage sludge, and implementation of decentralized treatment methods etc. have gained significant traction in recent years. These initiatives targeted to make our cities sustainable are important. On the other hand, measuring the sustainable performance of essential services of a city in light of changing affecting its ecological footprint is equally important. This requires building of a computational modeling framework using holistic systems analysis tools in combination with mathematical and statistical techniques. The project focuses on to measure and quantify the sustainable performance of essential services offered by city of Umeå using holistic approaches as LCA (Life Cycle Assessment) and LCC (Life Cycle Costing). These system analysis tools are used to evaluate alternate scenarios that can be tagged as "sustainable practice" compared to an already established practice of operating a city (e.g. what is sustainable performance of city of Umea if district heat requirements of the city are met/ waste forest biomass and municipal solid waste is diverted to produce biofuels?). The results are interpreted to develop generate a decision making framework that will allow stakeholders (e.g. municipalities) to make sustainably meaningful decisions in operating a city.

Facilities	Current Practices	Future Potential Practices
Waste Water Treatment Plant	Tertiary Treatment using FeCl <sub>3</sub>	Tertiary Treatment E-peroxone
	Sludge is Landfilled	Sludge to Land farming Sludge to incineration (Cement kilns) Biochar filters
Municipal Solid Waste (MSW) Plant	Organic waste to Biogas (Used in Heat/Electricity)	Biogas upgraded to be used in Transport Sector
	Residual MSW to Incineration	Upscaling of Fly ash which is currently landfilled
	Recycling routes	Alternate recycling options

Sustainable Assessments on the following waste services are expected to be performed during the thesis.

P-3

## Mesoporous melamine-formaldehyde. A potential solution for utilization of CO<sub>2</sub>?

<u>Thai Q. Bui</u><sup>1</sup>, Lakhya J. Konwar<sup>1</sup>, Ajaikumar Samikannu<sup>1</sup>, Jyri-Pekka Mikkola<sup>1</sup>

<sup>1</sup>Department of Chemistry, Umeå University, Umeå, Sweden <sup>2</sup>Department of Chemical Engineering, Åbo Akademi University, Åbo-Turku, Finland

Carbon dioxide  $(CO_2)$  utilization has attracted increasing attention worldwide for the sake of global warming mitigation. Moreover,  $CO_2$  could be a potential C1 source to produce industrial chemicals as it is a non-toxic, non-flammable, inexpensive raw material, available in bul-scale and a renewable resource. So far, direct synthesis of cyclic carbonates from epoxides and  $CO_2$  is one of the most promising routes for  $CO_2$  utilization due to 100% atom economy (no by-products). Moreover, their use in industrial applications as aprotic polar solvents, electrolytes for lithium-ion batteries, useful intermediates for production of pharmaceuticals and polymers are promising. Very recently, our group has developed renewable N-doped carbons from low-cost bio-waste precursors for direct carbonation of epoxides with  $CO_2$  to cyclic carbonates.<sup>1</sup> However, such carbon materials are still less active and experiments with fixed-bed reactor are still missing. Furthermore, in general, there are also limited reports in literature depicting the use of heterogeneous catalysts for production of cyclic carbonates from epoxides in continuous flow reactors under subcritical  $CO_2$  condition.

Herein, we report the catalytic application of the mesoporous melamine-formaldehyde catalyst in both batch and fixed bed reactors for direct production of cyclic carbonates from epoxides and CO<sub>2</sub> under mild conditions. The catalytic material was obtained for the first time through a HCl-catalyzed organic sol-gel process of N-rich precursor (melamine) with paraformaldehyde, followed by a hydrothermal treatment in an autoclave at 150°C for 24 hours. The catalytic material was characterized using standard techniques such as N<sub>o</sub> physisorption, temperature programmed desorption (TPD), CO<sub>2</sub> temperature programmed desorption (CO<sub>2</sub>-TPD), X-ray photoelectron spectroscopy (XPS). The material exhibited excellent catalytic activity upon direct carbonation of epoxides (epichlorohydrin, 1,2-butylene oxide, styrene oxide) with CO2 to cyclic carbonates under moderate temperatures (100-140 °C) and CO<sub>2</sub> pressures (13-20 bar). The catalytic conversion of CO<sub>2</sub> was performed without any other additives, solvents, metals, or co-catalysts. Most importantly, the low-cost, scalable polymer catalyst demonstrated excellent catalytic performance (activity, selectivity, stability) in continuous flow process under mild conditions, which made it potential material for CO<sub>2</sub> utilization in industrial scale.

#### Reference

<sup>1</sup>A. Samikannu, L. J. Konwar, P. Mäki-Arvela, J.-P. Mikkola (2019) Appl. Catal. B: Environ. Renewable N-doped active carbons as efficient catalysts for direct synthesis of cyclic carbonates from epoxides and CO<sub>2</sub> **241**: 41-51.

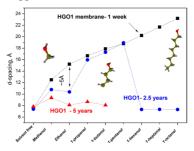
### P-4

## Strong effect of ageing on swelling properties of graphene oxide membranes in alcohols

<u>Artem Iakunkov</u><sup>1</sup>, Jinhua Sun<sup>1,2</sup>, Anastasia Rebrikova<sup>3</sup>, Mikhail Korobov<sup>3</sup>, Alexey Klechikov<sup>1,2</sup>, Alexei Vorobiev<sup>2</sup>, Nicolas Boulanger<sup>1</sup>, Talyzin A.V.<sup>1</sup>

<sup>1</sup>Department of Physics, Umeå University, Sweden <sup>2</sup>Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden <sup>3</sup>Department of Chemistry, Moscow State University, Moscow, Russia

The swelling of graphene oxide membranes aged over different periods of time (from 1 week to 5 years) was studied in alcohols row from methanol up to 1-nonanol using synchrotron radiation XRD. Membrane samples synthesized in 2013 and characterized at the moment using XPS, XRD and FTIR [1] were re-examined after 5 years of a storage at ambient conditions revealing a dramatic modification of the structure and swelling properties. Both precursor graphite oxides and freshly prepared Hummers Graphene Oxide (HGO) membranes were found to swell in the whole set of nine liquid alcohols with increase of interlayer spacing from  $\sim 7$ Å (solvent free) up to  $\sim 26$ Å (in 1-nonanol). At the same time the swelling of HGO membranes aged for 0.5-1.5 years become significantly smaller and completely disappeared for alcohol molecules larger than hexanol. Moreover, the HGO membranes stored at ambient conditions for 5 years showed nearly complete absence of swelling in all alcohols. In contrast, precursor graphite oxide powders showed the unmodified swelling in alcohols even after 4 years of the ageing. Remarkably, significant swelling of GO membranes in water was observed even after 5 years of the ageing. It was shown that the ageing starts on the surface of the multilayered structure and slowly penetrates into the deeper regions. Since the swelling defines size of permeation channels, the ageing effect is one of important parameters which could explain strong scatter in reported filtration/ separation properties of GO membranes. The time and conditions of air storage require standardization for better reproducibility of results related to performance of GO membrane in various applications.



### Fig. 1: GO membranes swelling in alcohols: Interlayer distance provided by d(001) for freshly prepared sample and samples stored on air for prolonged period of time

<sup>1</sup>Talyzin, A.V., et al., (2014) *Nanoscale* The structure of graphene oxide membranes in liquid water, ethanol and water-ethanol mixtures, **6**(1), 272-281.

P-5

### Hydrothermal pretreatment of sugarcane bagasse with and without sulfuric acid - New insights on effects of pretreatment severity

Dimitrios Ilanidis<sup>1</sup>, Stefan Stagge<sup>1</sup>, Leif J. Jönsson<sup>1</sup>, Carlos Martín<sup>1</sup>

<sup>1</sup>Department of Chemistry, Umeå University, SE-901 87, Umeå, Sweden

Lignocellulosic residues, such as sugarcane bagasse, have great potential for production of bio-based commodities, green chemicals, and advanced biofuels such as cellulosic ethanol. Lignocellulosic biomass is not easily biodegradable and the cost of cellulose-degrading enzymes is high. Thus, it is necessary to pretreat the lignocellulosic biomass as a part of the conversion process. Pretreatment of sugarcane bagasse was investigated using dilute-sulfuric acid (DA) and uncatalysed hydrothermal pretreatment (HT). The settings for temperature (175-205°C) and time (4-51 min) were varied in such a way that the severity factor was always maintained at one of three predetermined values. The analysis of either liquid phase after pretreatments covered monosaccharides and a large amount of inhibitors and gravimetric analysis of the solid phase were useful tools to investigate and understand how the temperature and time of both uncatalyzed and acid-catalyzed pretreatments affect the formation of inhibitors, the enzymatic digestibility of pretreated solids, and fermentability of pretreatment liquids.

The increase of temperature at constant severity factor pretreatments led to decreased pretreatment yields, higher degree of hemicellulose solubilization and formation of bioconversion inhibitors such as furan aldehydes, aliphatic acids, total phenolics, and benzoquinones. Glucose was the main sugar in DA liquors, while xylose was predominant in HT liquors. Acid-catalyzed and hydrothermal pretreatment showed different trends with respect to the effect of severity on furfural concentration. For a given severity factor, the concentration of furan aldehydes was directly proportional to the temperature for both pretreatment methods. This investigation also indicated that the enzymatic digestibility of pretreated cellulose increased increasing the temperature in HT whereas in DA the trend was opposite. The inhibition of cellulases by the pretreatment liquid increased with the severity, and was more significant for DA than for HT.

The investigation gives better understanding of fundamental aspects of hydrothermal pretreatment of sugarcane bagasse, and provides guidance for the development of a cost and energy-efficient hydrothermal pretreatment of sugarcane bagasse industrial process.

### P-6

## **CELLULOSE SYNTHASE INTERACTING 1** is required for wood morphogenesis and mechanics in aspen

<u>Anne Bünder</u><sup>1</sup>, O. Sundman<sup>2</sup>, A. Mahboubi<sup>3</sup>, S. Persson<sup>4</sup>, S. Mansfield<sup>5</sup>, M. Rüggeberg<sup>6</sup>, T. Niittylä<sup>1\*</sup>

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Cellulose biosynthesis is a highly regulated process, taking place at the plasma membrane. The alignment and incorporation of cellulose microfibrils in the cell wall shapes plant morphogenesis, cell size and influencing mechanical properties of cell walls and tissues. Cellulose microfibrils are synthesized by a CELLULOSE SYNTHASE COMPLEX (CSC) guided by cortical microtubules (MT). In Arabidopsis the CELLULOSE SYNTHASE INTERACTING PROTEIN1 (CSI1) is required for a MT-based guidance of CSCs during primary cell wall formation as well as during the initial phase of secondary cell wall patterning enabling a proper alignment of emerging cellulose microfibrils in the cell wall. Arabidopsis csi1 mutants show a delocalization of the CSCs from MTs affecting cell wall patterning in both primary and secondary cell wall. In hybrid aspen (*Populus tremula x tremuloides*) gene expression of the functional ortholog PtCSI1 is highly increased during secondary cell wall formation. We show that in hybrid aspen a reduction of *PtCSI1* causes impaired mechanical wood properties evident as a decrease in both the elastic modulus and ultimate stress in thin wood sections. Fibre dimensions and cellulose degree of polymerization (DP) were reduced in the CSI1RNAi mutant lines, while the secondary cell wall cellulose microfibril angle (MFA) was not affected. Our results suggest that besides in primary cell wall formation, a reduction of PtCSI1 also has an effect on wood secondary cell wall structure, supported by PtCSI1 gene expression, and impaired DP and wood mechanics.

P-7

### Generation of A Mucin Glycopeptide Microarray Library for Evaluation of Host-Pathogen Interactions

Sandra Behren<sup>1</sup>, J. Yu<sup>2</sup>, C. Pett<sup>1</sup>, M. Schorlemer<sup>1</sup>, U. Westerlind<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Umeå University, Umeå, Sweden <sup>2</sup>Department of Medicine, Imperial College London, London, United Kingdom

Mucins are heavily glycosylated proteins ubiquitously found on the epithelial cell surface in a membrane-bound or secreted form.<sup>1</sup> They contribute among other things to mucociliary clearance, an innate immune defense system which protects the airways against invading pathogens and chemical or physical stress factors.<sup>2</sup> Mucins exhibit extracellular tandem repeat (TR) regions rich in proline, threonine and serine (PTS) that form a scaffold for the attachment of *O*-linked glycans. Mucin *O*-linked glycans are often arranged in a multivalent fashion and function as ligands to different pathogens, which are cleared by the mucus under normal flow properties.<sup>3</sup> In airway diseases, mucin overexpression and altered terminal glycosylation, e.g. sialylation and fucosylation, as well as binding of pathogens to carbohydrate ligands, which leads to inflammatory-infective responses in the respiratory tract, occur.<sup>4-7</sup> This contributes to defect flow properties of the mucus and airway obstruction.

To better understand the role of mucin-type *O*-glycosylation in host-pathogen interactions, a synthetic glycopeptide library, immobilized onto microarray slides, was generated. For this purpose, a synthesis strategy was established to build-up diverse amino acid building blocks glycosylated with common mucin-type *O*-glycan core structures, which were subsequently introduced into mucin tandem repeat peptides by Fmoc-SPPS. To increase the diversity and generate specific glycan motifs, the glycan structures were further modified by chemoenzymatic elongation with N-acetyllactosamine structures, termination by 2,3- and 2,6-sialylation and fucosylation. The obtained glycopeptide library was then immobilized on microarray slides. The generated glycopeptide microarrays are currently employed in studies of bacterial and virus lectin binding preferences.

#### References

<sup>1</sup> Dekker J., Rossen J. W., Büller H. A., Einerhand A. (2002) *Trends in Biochemical Sciences* **27**: 126-131.

- <sup>2</sup> Thornton D. J., Sheehan J. K. (2004) Proc. Am. Thorac. Soc. 1: 54-61.
- <sup>3</sup> Rose M. C., Voynow J. A. (2006) Physiol. Rev. 86: 245-278.
- <sup>4</sup> Venkatakrishnan V., Packer N. H., Thaysen-Andersen M. (2013) Expert Rev Respir Med 7: 553-576.
- <sup>5</sup> Pett C., Schorlemer M., Westerlind U. (2013) Chem. Eur. J. 19: 17001-17010.
- <sup>6</sup> Pett C., Westerlind U. (2014) Chem. Eur. J. 20: 7287-7299.
- <sup>7</sup> Pett C., Cai H., Liu J., Palitzsch B., Schorlemer M., Hartmann S., Stergiou N., Lu M., Kunz H., Schmitt E., Westerlind U. (2017) *Chem. Eur. J.* **23**: 3875-3884.

### P-8

### Implementation of machine learning for more comprehensive process understanding in wastewater treatment plant

Dong Wang<sup>1</sup>, Nabil Souihi<sup>1</sup>, Lili Jiang<sup>2</sup>, Mats Tysklind<sup>1</sup>

<sup>1</sup>Department of Chemistry, Umeå University, SE 90187 Umeå, Sweden <sup>2</sup>Department of Computing Science, Umeå University, SE 90187 Umeå, Sweden

Online probes are used along the process line of the largest wastewater treatment plant (WWTP) in Umeå, and big historical data has been collected for the process parameters. To obtain a more comprehensive understanding of the processes besides the empirical knowledge, the random forest (RF) and deep neural network (DNN) models were built, tuned, and tested using the data before the effluent as the input and each effluent parameter (total suspended solid (TSS) and phosphate and polyphosphate (PO4)) as the outputs. With its extraordinary prediction performance, DNN was used in this study as the reference for RF even though it is much less interpretable compared to RF. The importance of the variables was evaluated by the Variable Importance Measures (VIM) and the way they influenced the output was demonstrated by the Partial Dependence Plot (PDP) after determining the optimal RF model.

 $R^2$  was used as the metric to indicate the regression performance. The (Training, Testing)  $R^2$  values for TSS were (0.934, 0.920) of RF and (0.935, 0.920) of DNN, while the ones for PO4 were (0.905, 0.886) of RF and (0.904, 0.872) of DNN. The results showed that for both TSS and PO4, the performances of RF and DNN were great and analogous to each other respectively – even the RF model showed slightly better performance on test data compared to the DNN model. This indicated that the RF model was reliable to be used to do further interpretation – VIM and PDP.

The VIM results showed that for both TSS and PO4, the temperature of influent was the most important variable, and TSS in the last return sludge pipe and the last second aeration basin were important as well. Besides, the flow rate of the second return sludge pipe was important for TSS. What's more, the TSS in the last three aeration basins were important for effluent PO4, which meant the effluent PO4 was highly dependent on the content of TSS in the aeration basins.

The PDPs of the top three most important variables for both TSS and PO4 were demonstrated to get the insight of how they influenced the outputs. The possible chemical, biochemical, physical, or engineering mechanisms behind these influences were discussed as well.

P-9

### Marine microorganisms for bioplastic production

Piotr Jablonski<sup>1</sup>, Mikkel Christiansen<sup>2</sup>, Hilde Hansen<sup>2</sup> and Knut Irgum<sup>1</sup>

<sup>1</sup>Umeå University, Department of Chemistry, Umeå, Sweden <sup>2</sup>Department of Chemistry, UiT – The Arctic University of Norway, Tromsø, Norway.

Can you imagine the world around you without petroleum-based plastics? Modern lifestyle promotes the usage of plastics in almost all areas of our lives. The global plastic production exceeds 330 Mt per year, causing massive environmental pollutions and degradations. Industry began to change the interest into biodegradable plastics, which can be biologically produced. Currently the cost of bioplastics production is high, making them less competitive with petroleum based products.

Our project is mainly focused into Polyhydroxyalkanoates (PHA), which are produced by many bacteria species. PHA are polyesters, having attractive and diverse material properties. The synthesis of PHA depends from different factors of which high carbon/ nitrogen ratio is the most prominent acting as a carbon storage mechanism, when excess carbon is available for the bacteria to store as an energy reserve. Some bacteria species are known to store more than 90 % PHA of the cell dry weight.

Bacteria sampled from Norwegian and Black Sea have been tested and growth optimized for PHA production by FT-IR and GC-MS analyses. Our focus is now on developing a new downstream process, significantly reducing the costs of production and increasing competitiveness with petroleum based plastics. We are testing several different extraction and recovery techniques, with the help of environmental friendly solvents. One of the assumptions is to produce monomers as a final product, making the process resistant to fluctuations in biosynthesized polymer. The ultimate project goal is to prepare fully upscalable industrial process in accordance to the green chemistry principles.

### P-10

### Morphological Analysis of Apolipoprotein E Binding to Aβ Amyloid Using a Combination of Surface Plasmon Resonance, Immunogold Labeling and Scanning Electron Microscopy

<u>Tohidul Islam</u><sup>1</sup>, Anna L. Gharibyan<sup>1</sup>, Cheng Choo Lee<sup>2</sup> and Anders Olofsson<sup>1\*</sup>

<sup>1</sup>Department of Medical Biochemistry and Biophysics. Umeå University, SE-901 87, Umeå, Sweden

<sup>2</sup>Umeå Core Facility for Electron Microscopy (UCEM), Umeå University, SE-90187, Umeå, Sweden

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Immunogold labeling in combination with transmission electron microscopy analysis is a technique frequently used to correlate high-resolution morphology studies with detailed information regarding localization of specific antigens. Although powerful, the methodology has limitations and it is frequently difficult to acquire a stringent system where unspecific low-affinity interactions are removed prior to analysis. We here describe a combinatorial strategy where surface plasmon resonance (SPR) and immunogold labeling are used followed by a direct analysis of the SPR-chip surface by scanning electron microscopy. Using this approach, we have probed the interaction between Aß amyloid fibrils, associated to Alzheimer's disease, and apolipoprotein E (ApoE), a well-known ligand frequently found co-deposited to the fibrillar form of Aβ *in vivo*. The results display a lateral binding of ApoE along the amyloid fibrils and illustrates how the gold-beads represent a good reporter of the binding. This approach exposes a technique with generic features which enables both a quantitative and a morphological evaluation of a ligand-receptor based system. The methodology mediates an advantage compared to traditional immunogold labeling since all washing steps can be monitored and where a high stringency can be maintained throughout the experiment.

Keywords: Aβ; ApoE; immunogold labeling; SPR; SEM; fibrils; morphology

P-11

## Fungal community responses to clear-cutting and addition of nitrogen to seedlings

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<sup>1</sup>Umeå Plant Science Centre, Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, Sweden

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<sup>3</sup>Department of Forest Ecology and Management, Swedish University of Agricultural Sciences, Sweden.

Ectomycorrhizal associations are key to plant nutrient dynamics in boreal systems, through both active involvement in decomposition and nutrient uptake and transport to host plants. Understanding the nature of mycorrhizal associations is therefore vital to understanding these forests. Mycorrhizal associations are complex because there is a vast array of plant and fungal species involved, each pair of which may have a separate relationship, and which may change depending on field conditions. In general, the fungal species provide the plant with mineral nutrients in exchange for fixed carbon skeletons. The end cycle of forest management involves the removal of mature trees through clear-cutting, followed by soil scarification and either the planting of nursery grown seedlings or direct sowing of select seed. However, this management approach can impair soil health through mineral losses, particularly nitrogen, and through enrichment of saprotrophic species and depletion of plantassociated fungi - leading to poorer seedling establishment and reduced seedling growth. This represents a challenge for forestry. In response to this challenge, new re-planting methods have been developed to produce high quality seedlings. One of these is the seedPAD, a germination matrix containing seed from seed orchards that can be used in combination with fertilizers. Using plant and soil DNA metabarcoding and amplicon sequencing, we analyzed the effect of clear-cutting and soil scarification on the soil fungal community, and on the subsequent recruitment of fungal species by germinating seedlings. In addition, we used seedPAD's containing either organic or inorganic N-sources to assess the effect of supplemental N-addition on seedling germination, growth and fungal recruitment by the germinating seedlings.

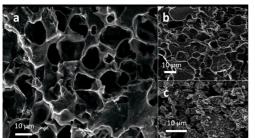
### P-12

## Activated graphene as electrode material in supercapacitors

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Supercapacitors are energy storage devices with high power density, but insufficiently high energy storage density. It is generally assumed that high specific surface area (SSA) is advantageous for electrode material in supercapacitor. Activated reduced graphene oxide (a-rGO) materials<sup>1</sup> were prepared using activation temperatures 550 °C - 850 °C providing SSA in the range 2000 m<sup>2</sup>/g - 3000 m<sup>2</sup>/g. Another set of samples was produced by ball milling of a-rGO with  $3000 \text{ m}^2/\text{g}$  to improve the bulk density of the material (Fig. 1). The porosity of materials was characterized using analysis of nitrogen and water sorption isotherms. The performance of electrodes prepared using a-rGO materials was evaluated in supercapacitor cell in 6 M KOHelectrolyte. It was found that ball milling results not only in five-fold increase in bulk density, but also in collapse of mesopores and preparation of microporous material. It was also found that the pore size distribution was quite different for materials prepared at different activation temperatures. The best gravimetric and volumetric capacitance was achieved not for samples with the highest value of BET SSA, but for materials which demonstrate a delicate balance of hydrophilicity, micropore volume and better conductivity. Remarkably, the highest capacitance was observed for



materials with similar pore size distribution but produced by two rather different methods. The highest capacitance (~170 F/g) was found for the sample produced at 550 °C. Light ball milling was found to improve the gravimetric capacitance. Stronger ball milling results in breakup of 3D porous structure and decrease of the N2 SSA.

Fig. 1. SEM images of (a) pristine reference sample of showing large micrometer sized voids; (b) a-rGO activated at 550 °C and c) reference sample after 30 minutes of ball milling. It can be seen that larger pores has been destroyed by the milling.

#### Acknowledgements

Authors acknowledge funding from the European Union's Horizon 2020 research and innovation program under grant agreement No785219 and the Swedish Research Council grant (no. 2017-04173). M.K. acknowledge support by RFBR grant № 18-33-00439. A.I. and A.T. acknowledge support from Kempestiftelserna. A.T thanks COST Action CA 15107 "Multi-Functional Nano-Carbon Composite Materials Network (MultiComp). We acknowledge also support by Vibrational Spectroscopy Platform of Umeå, University and A. Shchukarev for technical support with XPS.

#### References

<sup>1</sup> Klechikov A. et al. (2015) *Chemical Communications* **51**(83): 15280-15283.

## Information from Infrastructures

### I-13

### 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 cuttingedge 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)
- Leica SP8 Falcon Confocal (KBC building, A4)
- Leica SP8 Confocal (Molecular biology Department)
- Bruker Atomic Force Microscope (KBC building, H6)
- Biacore 3000 (KBC Building, A5)
- Auto-ITC<sub>200</sub> (KBC Building, A5)
- Proteon XPR36 (KBC Building, A5)
- Ligand Tracer<sup>®</sup> 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, <u>richard.lundmark@umu.se</u> Facility Manager: Irene Martinez Carrasco, <u>irene.martinez@umu.se</u> Senior Research Engineer for CLEM: Naga Venkata Gayathri Vegesna, <u>gayathri.vegesna@umu.se</u>

#### MORE INFORMATION

https://www.umu.se/en/research/infrastructure/biochemicalimaging-centre-umea-bicu/



### 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<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O)
- TOC analyzer (also including particulate carbon)
- Nutrient analyzer (NO3+NO2, NH4, PO4, TN, TP)
- Fluorometer
- Liquid scintillation counter (<sup>3</sup>H, <sup>14</sup>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



#### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/baf/

### I-15

### **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 and starch detection

• Size exclusion chromatography (SEC) for determination of MW, DP etc. of lignocellulose polymers

### CONTACT

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

### MORE INFORMATION

 $\label{eq:https://www.upsc.se/platforms/cell-wall-analysis/4845-biopolymer-analytical-platform.html$ 

### **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: <u>erik.chorell@umu.se</u> Stina Berglund Fick: <u>stina.berglund.fick@umu.se</u>

### MORE INFORMATION

www.cbcs.se; www.scilifelab.se/facilities/cbcs; www.umu.se/en/research/infrastructure/cbcs/



### I-17 I-18

### **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?** 

### CONTACTS

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

### **MORE INFORMATION**

https://www.umu.se/en/umea-marine-sciences-centre/



### 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, UVcuring 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<sub>2</sub>, Ar, H<sub>2</sub>, O<sub>2</sub>, liquid CO<sub>2</sub>, 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 or Nanolab homepage 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

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

### MORE INFORMATION

https://www.umu.se/en/research/infrastructure/nanolab/



### I-20

### Nuclear Magnetic Resonance – NMR for Life

The KBC Core facility NMR provides access to state-of-the-art NMR equipment and exper- tise for all researchers in the KBC and Campus environment. This infrastructure is part of the national infrastructures "NMR for Life" (www.nmrforlife.se), funded by KAW and ScilifeLab and operated by the Swedish NMR Centre at the University of Gothenburg and Umeå University. As part of "NMR for Life", the infrastructure grants access to academic and industrial researchers across Sweden.

The NMR facility offers access to powerful liquid and solid-state NMR infrastructure with in Umeå instruments at 850, 600, 500 and 400 MHz. High-field instruments are equipped with cryo-probes for optimal sensitivity for biomolecular solution NMR and environmental NMR. Robotic sample preparation and sample changers are available for high-throughput applications such as metabolomics of biofluids and fragment-based screening (FBS). This facility offers nationwide unique solid-state NMR at 850 and 500 MHz for studies of membrane proteins & amyloid fibrils and metabolomics on intact tissues.

### SERVICE PROVIDED BY THE INFRASTRUCTURE

"NMR for Life" offers nation-wide NMR access in three areas: Liquid- and solidstate structure analysis, metabolite studies and chemical biology. In addition, we offer expert assistance throughout a project. Three-dimensional structures can be determined for soluble proteins, solid and membrane-bound proteins, nucleic acids and biomolecular complexes.

Metabolite studies, especially metabolomics, can be carried out on liquid and solid samples, including temperature-sensitive biological specimen. Advanced support of the entire process is provided, including bioinformatics data analysis support (through NBIS). Through close collaboration with the Swedish Metabolomics Centre, we offer combined NMR- and MS-based metabolomics.

Our solid state NMR equipment allows structural studies of insoluble protein aggregates such as amyloid fibrils and membrane proteins in their functional lipid environment. FBS is routinely performed using substance libraries from - and in interaction with - Chemical Biology Consortium Sweden (CBCS) and Laboratories for Chemical Biology Umeå (LCBU).

### PERSONNEL

Gerhard Gröbner, prof., Platform Director, Dept of Chemistry Jürgen Schleucher, prof., Platform Director, Dept of Med Biochemistry and Biophysics Mattias Hedenström, Senior Research Engineer, Dept of Chemistry Tobias Sparrman, Senior Research Engineer, Dept of Chemistry Ilona Dudka, Senior Research Engineer, Dept. of Chemistry

Joao Figueira, Senior Research Engineer, Dept. of Chemistry

### STEERING COMMITTEE

Bernt Eric Uhlin, Prof., Dept Molecular Biology, MIMS and UCMR Fredrik Almqvist, Prof., Dept. of Chemistry

Pernilla Wikström, Prof., Dept. of Medical Biosciences

#### **MORE INFORMATION**

www.umu.se/en/research/infrastructure/nmr/ www.nmrforlife.se



### **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: <u>mikael.lindberg@umu.se</u>

### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/pep/



### **Swedish Metabolomics Centre - SMC**

Swedish Metabolomics Centre (SMC; <u>www.swedishmetabolomicscentre.se</u>) 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

### CONTACTS

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

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

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

### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/metabolomics/: https://www.swedishmetabolomicscentre.se/



### **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.

### CONTACTS

The facility is located on the 6:th floor in the KBC building. Peter Haglund Director, 090-786 6667 Main Contact: Co-ordinators: Erik Biörn ICP-MS, 090-786 5198 Peter Haglund Non-Target MS Analysis, 090-786 6667 Per Lilielind GC-MS, 090-786 9321 Richard Lindberg LC-MS, 090-786 5464 Dmitry Shevela Isotope-ratio MS, 090-786 5293

### MORE INFORMATION

https://www.umu.se/en/research/infrastructure/tap/: http://tap.chem.umu.se/



## I-23 I-24 I-25

### **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 facility labs, where students and scientists can perform advanced sample preparation, imaging and image analyzes.

SEM instruments, 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 methodology and thin lamella preparation for subsequent TEM or tomography analyses.

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. The method "Cryo-EM single particle 3D reconstruction" is used for structure biology studies and cryo-electron tomography is used to study e.g. molecular complexes, subcellular volumes or microorganisms in 3D.

Together with the BICU, UCEM provides CLEM imaging support as part of the National Microscopy Infrastructure (NMI) and have during 2019 installed a new fluorescence microscope with a cryo sample stage. The cryo-EM facility is a SciLilfeLab node and part of CryoNET. UCEM also support sample preparation for MAX IV microscopy beamline users. The establishment of an advanced EM facility in Umeå was made possible through external funding by the Swedish Research Council, Knut and Alice Wallenberg Foundation and the Kempe Foundations.

### CONTACTS

For general enquiries: Linda Sandblad, Facility Coordinator / Head of Facility

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

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### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/umea-core-facility-for-electron-microscopy-ucem/



### 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 second one is being purchased), 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, *in vivo* chemical compositional analysis of tissues). 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).

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#### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/visp/



### 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  $\ensuremath{\mathbb{R}}$  , 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-K $\alpha$  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 $(\mathbb{R})$ )
- 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

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### MORE INFORMATION

https://www.biostruct.umu.se/facilities/x-ray-facility/



### 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 K $\alpha$  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:

- $\bullet$  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.)
- $\bullet$  Non-destructive elemental depth profile 10 nm into the sample and surface heterogeneity assessment
- $\bullet$  Lateral variations in surface chemical composition (XPS imaging with spatial resolution of 5  $\mu\text{m})$
- 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)

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### **MORE INFORMATION**

https://www.umu.se/en/research/infrastructure/xps/



### The Single Cell Detection Facility: Fluorescence *In Situ* Hybridization (FISH)

for environmental, clinical, food and biotechnology research

The goal of the Single Cell Detection Facility is to employ Fluorescence In Situ Hybridization (FISH) to identify genes in intact whole cells or viruses in their natural environment - without cultivation nor nucleic acid extraction. FISH can therefore complement not only other microscope based studies (e.g. fluorescence microscopy, electron microscopy), but also disruptive molecular biological methods, which rely on the extraction of cell components such as DNA. Thus, FISH can retrieve the information that is lost when extracting cell components, 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 certain viruses. The most common gene target for cell identification is the ribosomal gene, but new techniques are emerging that will also allow the in situ detection of other genes, such as housekeeping genes, functional genes, and pathological genes. FISH can also be combined with many other methods, such as cultivation, molecular methods, radioactive/isotope methods, flow cytometry, RAMAN spectroscopy, mass spectrometry, and 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 contains all equipment necessary for FISH, including a large collection of gene probes for various taxa, reference samples, anda 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 at UmU and outside, 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. Within the near future, two kinds of courses will be organized at KBC: a) introduction into the bioinformatic package ARB for phylogeny and biomarker design; b) overview of different FISH techniques for different research fields (environmental, clinical, industrial).

### CONTACT

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• Lee NM. 2019. Whole Cell Identification of Microorganisms in their Natural Environment with FISH. Analytical Geomicrobiology. Cambridge University Press. Eds: D Alessi, H Veeramani, J Kenney, pp. 187-212.

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

#### **MORE INFORMATION**

Homepage will be launched November 2019

Overview Infrastructure Presentations				
Scientific Infrastructure	Contact persons	Tour	Panel discussion	Poster
Biochemical Imaging Centre Umeå (BICU)	richard.lundmark@umu.se irene.martinez@umu.se	yes	yes	I-13
Biogeochemical Analytical Facility (BAF)	ann-kristin.bergstrom@umu.se anders.jonsson@umu.se			I-14
Biopolimer Analytical Platform (BAP)	totte.niittyla@slu.se junko.TS@slu.se			I-15
Computational Life Science Cluster (CLiC), NBIS	johan.trygg@umu.se jeanette.tangrot@umu.se allison.churcher@umu.se		yes	I-29
Chemical Biology Consortium Sweden (CBCS)	stina.berglund.fick@umu.se erik.chorell@umu.se	yes	yes	I-16
Technical platforms at Umeå Marine Sciences Centre	siv.huseby@umu.se henrik.larsson@umu.se	yes*	yes	I-17, I-18
NanoLab	roushdey.salh@umu.se			I-19
Nuclear Magnetic Resonance Core Facility (NMR)	mattias.hedenstrom@umu.se tobias.sparrman@umu.se jurgen.schleucher@umu.se gerhard.grobner@umu.se	yes	yes	I-20
Protein Expertise Platform (PEP)	mikael.lindberg@umu.se		yes	I-21
Swedish Metabolomics Centre (SMC)	annika.johansson01@umu.se	yes	yes	
Trace Analysis Platform (TAP)	peter.haglund@umu.se			I-22
Umeå Core Facility for Electron Microscopy (UCEM)	linda.sandblad@umu.se	yes	yes	I-23, I-24, I-25
Vibrational Spectroscopy Core Facility (ViSp)	andras.gorzsas@umu.se	yes	yes	I-26
X-Ray Crystallization Platform (X-ray)	uwe.sauer@umu.se		yes	I-27
X-Ray Photoelectron Spectroscopy (XPS)	andrey.shchukarev@umu.se			
Fluorescence In Situ Hybridization facility (FISH)	natuschka.lee@umu.se	**	yes	I-28
* A guided tour will be arranged later if enough people sign up at the registration desc				
** A discussion table in the KBC Cafeteria				

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KBC Service Centre	servicecenter.kbc@umu.se
KBC Printing service	lars.aberg@umu.se
Mechanic workshop at the Department of Physics	peter.wikstrom@umu.se isak.silander@umu.se
KBC IT-support (CAS Login)	http://kbc-support.ad.umu.se/IT/
KBC Chemical Store (CAS login)	https://chemshop.chem.umu.se

## MORE INFORMATION ABOUT COORDINATED SERVICES AT KBC



https://www.umu.se/en/chemical-biological-centre/services-kbc/

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