KBC
CHEMICAL BIOLOGICAL CENTRE

KBC DAYS 2023

7-8 November

Programme - Research Infrastructures -
PhD student presentation abstracts - Participants

UMEÅ UNIVERSITY

SLU

DAY 1, Tuesday 7 November

SESSION 1
Chairperson: Stefan Björlund

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

9.05 **Opening of the KBC DAYS 2023**
Mikael Elofsson
Dean, Faculty of Sciences and Technology, Umeå University

9.15 **Tribute to Carl Kempe**
Gunnar Öquist
Professor Emeritus, Department of Plant Physiology, Umeå Plant Science Centre, Umeå University

9.30 **IceLab and the Center for modeling adaptative mechanisms in living systems under stress**
Martin Rosvall
Director of IceLab, Department of Physics, Umeå University

9.45 **AI-assisted deep learning segmentation and quantitative analysis of X-ray micro tomography data**
Anna Strandberg
Departement of Applied Physics and Electronics, Umeå University

10.00 **Studying microbial communities from past and present aquatic systems with environmental DNA**
Eric Capo
Department of Ecology and Environmental Science, Umeå University

10.15 *coffee break*

SESSION 2: NEW FACULTY MEMBERS, AWARDS and GRANT RECIPIENTS from KBC
chairperson: Nasim Sabouri

10.35 **A unique light source to realize miniature particle accelerators and film electron motion in matter**
László Veisz
Relativistic Attosecond Physics Laboratory (REAL), Department of Physics, Umeå University

10.50 **Innovative treatment for extrapulmonary benefits in COPD**
André Nyberg
Department of Community Medicine and Rehabilitation, Umeå University

DAY 1, Tuesday 7 November

11.05 **The AI Council of the Faculty of Medicine, UmU: Vision, long-term goals, strategic action plan and activities**
Jenny Persson
Chair of the Faculty of Medicine's Council for AI and Autonomous Systems

11.15 **The ageing chaperome - from phenotype to functionality**
Verena Kohler
Department of Molecular Biology, Umeå University

11.30 **Ultrafast nanoscience: from understanding the structure and function of materials and molecules to next generation technologies using light**
Nicolò Maccaferri
Department of Physics, Umeå University

10.45 **Light harvesting in the world's most cosmopolitan algae**
Heidi Burdett
Department of Ecology and Environmental Science, Umeå University

12.00 *Lunch break*

Session 3: NEW FACULTY MEMBERS, AWARD and GRANT RECIPIENTS from KBC and ELEVATED TALKS PRESENTATIONS by PhD STUDENTS
Chairperson: Micael Jonsson

13.00 **Prisutdelning för att fira Bror Holmbergs medalj till Knut Irgum /Award ceremony to celebrate Bror Holmbergs medalj awarded to Knut Irgum**
Hans Adolfsson
Vice-chancellor, Umeå University

13.10 **Aboveground-Belowground Linkages and Global Changes**
David Wardle
Department of Ecology and Environmental Science, Umeå University

13.25 **Elevator talks presentations by PhD students (Part I)** (2 min each)

• Metabolic cooperation of bacteria within dual-species biofilms and their connection with catheter-associated urinary tract infections (Poster #1)
Dmytro Sokol, *Department of Chemistry, Umeå University*

• Unraveling mechanisms of how a gut commensal modulates Western diet-induced colonic mucus defects (Poster #2)
Sandra Holmberg, *Department of Molecular Biology, Umeå University*

• Salvaging dNTPs for mtDNA rescue (Poster #3)
Ololade Awoyomi, *Department of Medical Biochemistry and Biophysics, Umeå University*

13.35 **Plant science for a sustainable green transformation of the subarctic**
Stefan Jansson
Department of Plant Physiology, Umeå Plant Science Centre, Umeå University

13.50 **Elevator talks presentations by PhD students (Part II)** (2 min each)

• Ultra Structural Characterization of Cell Adhesion in Plants (Poster #4)
Özer Erguvan, *Department of Forest Genetics and Plant Physiology, Umeå Plant Science Centre, Swedish University of Agricultural Sciences*

• The combination of gallium citrate with linezolid or levofloxacin enhances the inhibition of the growth of drug-resistant Mycobacterium tuberculosis and results alterations in the metabolome
Oleksandr Ilchenko, *Department of Chemistry, Umeå University*

• Unlock biomass potentials!
Chaojun Tang, *Department of Chemistry, Umeå University*

• Enhancing Generalization in Clustered Collaborative Learning through Objective Inconsistency
Godwin Tunze, *department of Applied Physics and electronics*

INTERACTION SESSION

14.00 **Poster presentations by PhD students**

coffee

SESSION 4: PRESENTATIONS AND KEYNOTE LECTURE I

Chairperson: Nikola Zlatkov Kolev

15.00 **Keynote lecture I: AI in Biomedicine**
Prof. Dr. Mark B. Gerstein
Yale University, USA

16.00 **Students and teachers in the center- my experience as a teacher and director of studies**
Caroline Blomquist
Department of Ecology and Environmental Science, Umeå University

DAY 1, Tuesday 7 November

16.10 **Quality control of mitochondrially encoded proteins**
Andreas Kohler
Department of Medical Biochemistry and Biophysics, Umeå University

16.25 **Functional proteomics of human gut microbiome species**
Andre Mateus
Department of Chemistry, Umeå University

16.40 *poster viewing and mingle before the dinner starts*

18.00 *Dinner*

- Announcement of the PhD student presentation prize winners

DAY 2, Wednesday 8 November

SESSION 5: Innovative inspiration AND KEYNOTE LECTURE II
Chairperson: Stephan Wenkel

8.45 **Innovative inspiration: Opportunities with research in Umeå**
Johan Hedengran
Business Developer at Uminova Innovation, Umeå

9.00 **Keynote lecture II: Large language models in biology**
Assoc. Prof. Marek Mutwil
School of Biological Sciences, Nanyang Technological University, Singapore

9.45 *Coffee break*

SESSION 6: UMEÅ POSTDOC SOCIETY (UPS)
Chairperson and moderator: Pallabi Sengupta

10.00 **Introduction of Umeå Postdoc Society: activities and aims**
Maximiliano Estravis Barcala
President of the Umeå Postdoc Society

10.10 **Science communication and Grant writing**
Speaker:
Simone Wenkel**,** *Research Support and Collaboration Office, Umeå University*

Panel members:
Atin Sharma*, Department of Molecular Biology, Umeå University*
Selma Dahmane, *Senior Research Engineer, Department of Medical Biochemistry and Biophysics*

10.55 *Break*

11.00 **Transition from Academia to Industry**

Speaker:
Pia Keyser, *Business coach, Umeå Biotech Incubator*

Panel members:
Joanna Porankiewics Asplund, *Agrisera Antibodies*
Sofia Mayans,*Innovation and Business advisor, SLU holding*
Lotta Edvinsson*, Team manager/senior consultant, Knightec*

INTERACTION SESSION

11.45 **Posters by research infrastructures**

and standing lunch

DAY 2, Wednesday 8 November

SESSION 7: INFRASTRUCTURE PRESENTATIONS

Chairperson: Linda Sandblad

13.00 **Introduction**
Linda Sandblad
Director of Umeå Centre for Electron Microscopy (UCEM) and SciLifeLab Site Umeå, Department of Chemistry , Umeå University

13.10 **MAXS- Multi-purpose adaptive X-ray scateering platform for a broad user community**
Nils Skoglund
Department of Applied Physics and Electronics, Umeå University

13.20 **BioMolecular Characterization Unit (BMCU) - New research infrastructure at KBC**
Johan Olofsson Edlund
Department of Medical Biochemistry and Biophysics, Umeå University

13.30 **Protein Production in Plant Cells at the Protein Expertise Platform, PEP**
Uwe Sauer
Head of the Protein Expertise Platform. Department of Chemistry, Umeå University

13.40 **Atomic Force Microscopy**

Roushdey Sahl, *Director of NanoLab, Department of Physics, Umeå University*

Fouzia Bano, *Department of Clinical Microbiology, Umeå University*

Stephane Verger, *Department of Plant Physiology, Umeå Plant Science Centre, Umeå University*

14.05 *Coffee break*
and time to talk to infrastructures' representatives by their poster

SESSION 8: NEW FACULTY MEMBERS, AWARD AND GRANT RECIPIENTS AT KBC

Chairperson: Madeleine Ramstedt

14.15 **MIMS, Recent developments and future directions**
Anna Överby Wernstedt
Deputy Director of Molecular Infcetion Medicine Sweden (MIMS), Department of Molecular Biology, Umeå University

14.30 **Shining Light on Viral Assembly and Replication through Structural Biology**
Max Renner
Departement of Chemistry, Umeå University

DAY 2, Wednesday 8 November

14.45 **Machine learning approaches for novel secondary metabolite discovery**
Laura Carroll
DDLS Fellow, Department of Clinical Microbiology and Molecular Infetion Medicine Sweden (MIMS), Uneå University

15.00 **Light-emitting Electrochemical Cells: Basic Understanding for Practical Devices**
Ludvig Edman
Department of Physics, Umeå Univeristy

15.15 **Bacterial pore-forming proteins: ancient, but not out of fashion**
Aftab Nadeem
Department of Molecular Biology, Umeå University

15.30 **Concluding remarks**
Stefan Björklund
Scientific coordinator of KBC

- Announcement of the image contest prize winner

15.35 **Guided tours to infrastructures´facilities**

Keynote Speakers

Prof. Dr. Mark Bender Gerstein

PhD, Yale University, USA

(Albert L. Williams Professor of Biomedical Informatics, Professor of Molecular Biophysics and Biochemistry, of Statistics and Data Science, and of Computer Science; Co-director of the Yale Computational Biology and Bioinformatics program; Co-director of the Yale Center for Biomedical Data Science)

Prof. Gerstein obtained his B.A. in physics in 1989 from Harvard University and in 1993 earned a doctorate in theoretical chemistry and biophysics after studies of conformational change of proteins under the mentorship of Prof. Ruth Lynden-Bell and Prof. Cyrus Chothia at Cambridge University. From 1993 to 1996, Prof. Gerstein was a postdoctoral fellow in bioinformatics at Stanford University, guided by the 2013 Chemistry Nobel Laureate Prof. Michael Levitt. He came to Yale University in 1997 as an assistant professor.

Prof. Gerstein's research provides a comprehensive look at extremely complex and stochastic biological processes. Via mapping complex situations and their elements, he employs network analyses to establish a systems view of cells, whole organisms, and their populations. Thus, a central element (e.g., a protein or gene) is defined by its position in a network, the connectivity of which explains and predicts phenotypes and behaviors based on different hierarchies. To achieve that, his group has established a wide range of computational approaches based on data mining, machine learning, molecular simulation, and database design. His primary research interests include comparative and functional genomics (from personal genomics through disease and cancer genomics to neurogenomics), simulation of macromolecular structures and motions, and molecular network analysis. Biosafety is intimately linked to personal genomics and therefore an integral part of Prof. Gerstein's research interests—it is where security and molecular biology interplay, setting a new level of (bio)ethics.

Prof. Gerstein's laboratory developed significant tools and databases: the Database of Macromolecular Motions, tYNA, PubNET, PeakSeq and CNVnator. His research unit contributed to the development of scientific consortia, including ENCODE, modENCODE, 1000 Genomes projects, Brainspan and DOE Kbase. Prof. Gerstein is an AAAS fellow and a fellow of the International Society for Computational Biology. Among his awards and honors are the W. M. Keck Foundation Distinguished Young Scholars Award, and prizes from the US Navy, IBM, Pharmaceutical Research and Manufacturers of America, and the Donaghue Foundation.

Keynote Speakers

Assoc. Prof. Marek Mutwil

School of Biological Sciences, Nanyang Technological University, Singapore

Assoc. Prof. Marek Mutwil is a computational biologist with a Ph.D. from the University of Potsdam in 2011, Germany, and a Master's (2007) and Bachelor's (2005) degree in Biochemistry from the University of Copenhagen, Denmark.

He led the Regulatory Networks group at the Max Planck Institute of Molecular Plant Physiology, Germany (2012-2016). He has been serving as an Assistant Professor (2017-2022) and Associate Professor (2022-) at the Nanyang Technological University, School of Biological Sciences, Singapore.

His research is a fusion of experimental and computational methods, targeting plant evolution, specialized metabolism, and stress acclimation.

Information from Research Infrastructures

Umeå ancient DNA Lab

Analysis of environmental ancient DNA is a rapidly expanding scientific field, opening up exciting new possibilities to address paleoenvironmental, ecological and evolutionary research questions. To be able to conduct (environmental) ancient DNA research, the Department of Ecology and Environmental Science (EMG) established an ancient DNA (aDNA) lab at Umeå University in 2018.

Lab information

The aDNA lab is located in the basement of the Naturvetarhuset. This facility is divided into an entrance room (temporal storage of daily use lab material), a changing room (changing into clean suits, mask, etc.), and the operation lab (DNA extraction and PCR/ library preparation room).

• The aDNA lab counts with a positive air-pressure with HEPA filtering system at 40 l/s and it is equipped with UV sterilisation systems and alarms.

• The aDNA lab is equipped with a free DNA fridge (4°C) for reagent storage and a freezer (-20°C) for sample storage. Other materials include a biological hood, two spinners for 1.5-2 and 0.5 mL tubes, one centrifuge for 1.0-2.0 mL tubes, a UV crosslinker, an oven with rotators, a pre-PCR UV cabinet, a notebook computer, shelves, and working benches.

Tasks that can be performed at the Umeå ancient DNA lab

• DNA extraction from paleo- and environmental samples (such as soil, water, calciferous materials).

• aDNA and historical DNA storage

• Pre-DNA amplification (PCR) preparations

• Library preparation for metabarcoding and metagenomic analysis

CONTACT (lab managers)

Eric Capo: eric.capo@umu.se / +46(0) 733281450
Lourdes Martínez-García: lourdes.martinez.garcia@umu.se /+46(0)850521857
Department of Ecology and Environmental Sciences, Umeå University.

MORE INFORMATION
https://www.umu.se/en/research/infrastructure/adna-lab/

The Biogeochemical Analytical Facility - BAF

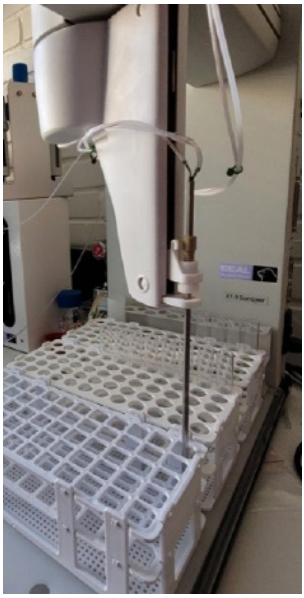
The infrastructure provides instruments for analysis of key chemical parameters in terrestrial and aquatic biogeochemical and ecological research and as such is of major interest for a large range of research groups.

BAF act as a core analytical facility for several major research projects run by researcher at EMG together with their collaborators and is also open 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, N_2O (FID, ECD)) - Perkin Elmer, Clarus 500
- TOC/TN analyzer (also including particulate carbon) - Skalar, Formacs HTI
- Nutrient analyzer (NO_3+NO_2, NH_4, PO_4, TN, TP) - Seal Analytical, QuAAtro -39
- Elemental analyzer, for analyses of C/N/H/S on solids and glass fibers. To be installed during November -23
-Elementar, Unicube
- Fluorometer - Perkin Elmer, LS55
- Flow cytometer - BD Instrument, Facs,Verse
- Respicond facility (to measure respiration)
- Inverted microscope also with epifluorescence and cameras - Nikon, Eclipse TE 2000 and Eclipse T*i*



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/

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.

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 and acetyl bromide lignin assay for lignin determination
- Enzymatic assays for soluble sugars and starch detection
- Size exclusion chromatography (SEC) for determination of MW, DP etc. of lignocellulose polymers
- Sample preparation and extraction using accelerated solvent extractor (ASE) 350

CONTACT

First contact for the customer: Laboratory manager, Junko Takahashi-Schmidt (Junko.TS@slu.se). We are in KBC G5

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, Professor, Dept. of Forest Genetics and Plant Physiology, SLU
Leif Jönsson, Dept. of Chemistry, UmU
Ola Sundman, Dept. of Chemistry, UmU
Stéphane Verger, Dept. of Plant Physiology, UmU
Junko Takahashi-Schmidt, Dept. of Forest Genetics and Plant Physiology, SLU

MORE INFORMATION

https://www.upsc.se/platforms/cell-wall-analysis/4845-biopolymer-analytical-platform.html

The Biochemical Imaging Centre Umeå - BICU

The Biochemical Imaging Centre Umeå (BICU) provides state-of-the-art imaging technology including advanced light microscopy and atomic force microscopy. BICU is an open-access imaging centre that offers cutting-edge technologies to researchers all over Sweden. Detailed information regarding our imaging centre organization and user fees can be found on our webpage.

We provide access and training to wide range of instruments including widefield, confocal and Tirf microscopy, FLIM, FLIM-FRET, FRAP and live cell imaging for an optimal spatial and temporal resolution. Furthermore, the centre provides access to Atomic Force Microscopy to generate topographical images and measure mechanical properties such as adhesion, stiffness and deformation of samples ranging from metal, glass, and surfaces coated with biomolecules to live cell

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 microscopy techniques and basic image analysis.

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 programs in microscopy. NMI in Umeå is the node specialized for advanced correlative imaging techniques. Hereby, BICU closely collaborates with Umeå Centre for Electron Microscopy (UCEM) to provide accessibility to various correlative light and electron microscopy (CLEM) techniques both in room temperature and cryo.

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

MORE INFORMATION

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

BioMolecular Characterization Unit - BMCU

Research Infrastructure BMCU is an interdisciplinary facility that provides state-of-the-art technology to characterize biomolecules. The facility allows measurement of affinity using different technologies, together with molecular weight analysis, folding and overall structure.

At the facility we offer access, training and consultation for the following instruments;

Isothermal Titration Calorimetry (ITC), Surface Plasmon Resonance (Biacore3000/ ProteOn), Quartz Crystal Microbalance with Dissipation (QCM-D), Mass Photometer and CD spectrophotometer.

CONTACTS

For questions about access and training:

Johan Olofsson Edlund

johan.olofsson.edlund@umu.se

Department of Medical Biochemistry and Biophysics

For questions about organization:

Ronnie Berntsson & Marta Bally

Ronnie.berntsson@umu.se

marta.bally@umu.se

MORE INFORMATION

https://www.umu.se/en/research/infrastructure/biomolecular-characterization-umea-/

Computational Analytics Support Platform - CASP

The Computational Analytics Support Platform (CASP) is a data analytics service at Umeå University (UmU), launched during 2021, within the framework of the Computational Life Science Cluster. CASP is a local co-funded KBC infrastructure that primarily supports, but also trains life scientists in the analysis of experimental data using data-driven tools and strategies. We focus on the analysis of data from a wide range of technologies including, but not limited to, downstream omics (metabolomics/ proteomics), spectroscopy and imaging.

Our aim is to help bridge the existing gap in data-driven life science, allowing researchers to convert complex data into meaningful biological and chemical interpretations via the use of advanced data-driven tools and strategies. Combined, the group have strong expertise in data-driven life science, in addition to wide domain expert knowledge arising from active engagement with multiple projects in the 'omics' area and beyond. This allows a full understanding of the researcher's needs, not only in terms of the data analysis, but also in how the data was generated and equally important, the interpretation of the biology behind the project.

Support packages we provide

- Packaged and customer-specific data analytics projects
- One-to-one consultations for data analysis support - long term
- Personalised tutorials including theoretical knowledge and hands-on experience using data analysis and processing software
- Extended data analytics support for high-throughput experimental platforms including the Swedish Metabolomics Centre

Services we provide

- Statistical experimental design
- Multivariate data analysis
- Image analysis
- Deep learning and machine learning
- Pathway analysis and interpretation
- Publishing

CONTACTS

Please contact the Platform Manager Kate Bennett (katie.bennett@umu.se). We can help with the analysis of many different data types so please feel free to contact us and we will be happy to answer your questions.
We look forward to supporting you in your projects!

MORE INFORMATION

https://www.umu.se/en/research/infrastructure/computational-analytics-support-platform-casp/

Chemical Biology Consortium Sweden - CBCS

CBCS aims to help researchers identify and develop small molecules that affect their biological system of interest. Using small molecules to decipher and understand the function of biological pathways can give you powerful research tools and set the ground for generating new leads for drug discovery. CBCS Umeå is part of the national SciLifeLab infrastructure service in Chemical Biology and has served researchers in Sweden for over ten years. Since 2022 the infrastructure has grown to include nodes at all six Universities and expanded the portfolio of new services to include, e.g., screening in BSL-3, cell painting and functional precision medicine. CBCS national services are available to all users.

CBCS Umeå offers research facilities, equipment, user clubs and staff with expertise in assay development, small molecule screening, medicinal and computational chemistry, and profiling of compound quality. In addition, we have a state-of-the-art compound collection for screening projects and a research collaboration with AstraZeneca that provides access for academic researchers to their annotated small molecule library of 14,000 compounds, targeting over 1,700 human proteins.

Consultations and smaller service projects are offered on a first-come, first-served basis, while more extensive screening and chemistry projects are made available through a peer-review process. Projects are prioritised based on merit, scientific impact, and practical feasibility. The instrument park at CBCS Umeå can be accessed through collaborative forms or user agreements.

EQUIPMENT AT CBCS UMEÅ

- Plate readers; Biotek Synergy H4 and BMG ClarioStar
- High Content Screening Microscope – Molecular Devises ImageXpress
- HIgh Throughput Flowcytometry - Sartorius IQUE3
- Liquid handling robotics; BC NxP, 96- and 384-wel, Wellmate
- HPLC, Gilson & Shimadzu, fully equipped chemistry labs

SERVICES PROVIDED

- Development of biological assays (e.g., baccteria, yeast, cells, organelles, viruses) for high-throughput screening
- Biochemical (target based) and cell-based high-hroughput screening
- High-throughput flow cytometry and imaging technology
- Organic chemistry and synthesis / Computational chemistry & modelling
- General expertise in preparative and analytical chemistry
- Course; Introduction to High Throughput Screening

CONTACTS

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Stina Berglund Fick: stina.berglund.fick@umu.se

MORE INFORMATION

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

High Performance Computing Center North - HPC2N

Are your simulations saturating your PC?: HPC2N as an alternative

High Performance Computing Center North (HPC2N) is a national center for Scientific and Parallel Computing.

The High Performance Computing Center North (HPC2N) is a local/regional resource for researchers at HPC2N's partners (IRF, LTU, Mittuniversitetet, SLU and UmU). National Data Science Node in ”Epidemiology and Biology of Infections” (DDLS). Our Director of HPC2N is Professor Paolo Bientinesi from the Computing Science Department.

We offer different types or hardware for computing and visualization including standard CPUs and Graphical Processing Units (GPU)s. Most common packages for Scientific Research are installed on our cluster for instance GROMACS, VASP, MATLAB, R/ Rstudio, among others.

To get started with our system, we offer different types of training courses including introductory courses, and more specialized courses in topics such as Molecular Dynamics, QM/MM, Git, R, Machine Learning, MPI, Julia, and OpenMP (recorded courses: : https://www.youtube.com/@HPC2N).

We provide a general support through a ticket system and a more advanced support for specific questions from researchers on-demand. .

CONTACT
For general questions: info@hpc2n.umu.se
Specific questions: support@hpc2n.umu.se

Visiting address:
Umeå University
MIT-building
HPC2N
Campustorget 5, 4th
S-907 36 Umeå
Sweden

MORE INFORMATION
https://www.hpc2n.umu.se/

NanoLab

NanoLab is an open-access infrastructure located at the Department of Physics. It is a classified Class 100 cleanroom which 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)**, **Four-Point Probe system , High Vacumm AFM,** as well as number of standard pieces of equipment, such as spin coaters, optical microscopes, vacuum ovens, hotplates, UV- curing boxes, analytical scales, etc. , visit NanoLabs website for more technical details, specific parameters and requirements for each individual equipment.

Original manuals and short user manuals for all equipment are to be found in KBC website and in the NanoLab.

The equipment in NanoLab is made available to all scientists at Umeå University, as well as external institutions. '

Besides the equipment available in the Nanolab, the Nanolab offers space for user´s own experiment inside the cleanroom. 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.

Trainings are offered 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 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. .

CONTACT

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

MORE INFORMATION

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

National Bioinformatics Infrastructure Sweden - NBIS

NBIS, National Bioinformatics Infrastructure Sweden, is a distributed national research infrastructure. We are the SciLifeLab bioinformatics platform and the Swedish node in Elixir, a European intergovernmental organisation bringing together life science resources from across Europe. With over a hundred staff members, we work with bioinformatics support, infrastructure and training.

NBIS has staff at six sites: Umeå, Uppsala, Stockholm, Linköping and Lund. We provide expertise in most areas of bioinformatics, including omics analysis, genome assembly/annotation, image analysis and biostatistics. We also offer support in systems development, such as interactive websites and data processing pipelines.

NBIS is mainly funded by the Swedish Research Council, SciLifeLab, the Knut and Alice Wallenberg Foundation, and Swedish universities.

We provide:

- Weekly online drop-in sessions, Tuesdays at 14:00; http://meet.nbis.se/dropin. Join to discuss study design, data analysis or other bioinformatics-related questions.
- Free consultation meetings to discuss study design.
- Hands-on project support, ranging from assistance with smaller tasks to long-term engagement.
- Free, extensive hands-on support to a limited set of projects selected in a peer review process (enabled by a grant from Knut and Alice Wallenberg Foundation).
- Tools, data management, systems development and guidelines for the life science community.
- Introductory and advanced training events, such as workshops in RNAseq data analysis, epigenomics data analysis, tools for reproducible research, python programming, and many other bioinformatics related topics.
- The Swedish Bioinformatics Advisory program - A mentorship program for PhD students interested in guidance from a bioinformatics expert.

CONTACT

For general questions: info@nbis.se
Local contact in Umeå: Jeanette Tångrot, jeanette.tangrot@umu.se

MORE INFORMATION

https://www.nbis.se

Nuclear Magnetic Resonance - NMR

The KBC NMR Core facility provides access to state-of-the-art NMR equipment and expertise for all researchers in the KBC and Campus environment. This facility is part of the national infrastructures SwedNMR funded by VR RFI and SciLifeLab and it is operated by the Swedish NMR Centre at the University of Gothenburg and Umeå University. As a national service infrastructure, we grant access to academic and industrial researchers across Sweden.

The NMR facility offers access to powerful liquid and solid-state NMR infrastructure with spectrometers ranging from 400 to 850 MHz. Our ultrafast magic angle spinning probe and cryo-MAS probe are unique for the Nordic countries, enabling high-resolution spectra of proteins and studies and complex biological samples in the solid-state. 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 and fragment- based screening (FBS).

SERVICE PROVIDED BY THE INFRASTRUCTURE

The NMR core facility offers nation-wide NMR access in four areas: Liquid- and solid-state structure analysis, materials science, metabolite studies and chemical biology. In addition, our personnel provide expertise according to the users need in all areas, from experimental design and sample preparation to data analysis.
Three-dimensional structures can be determined for soluble proteins, solid and membrane-bound proteins, nucleic acids and biomolecular complexes.
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 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 performed using substance libraries from - and in interaction with - Chemical Biology Consortium Sweden (CBCS).

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
João Figueira, Senior Research Engineer, Dept of Chemistry

MORE INFORMATION

https://www.umu.se/en/research/infrastructure/nmr/
https://www.scilifelab.se/services/integrated-structural-biology/
https://www.swednmr.se

Protein Expertise Platform - PEP

The Protein Expertise Platform (PEP) is a core facility at the Chemical Biological Center (KBC) and a node of the national infrastructure Protein Production Sweden (PPS). PEP provides researchers with needed services and expert advice in questions of bioinformatics, cloning, growth optimization, expression and protein purification

MATERIAL

PEP keeps a set of cloning vectors, with a variety of fusion partners and purification tags, designed to improve protein solubility and to facilitate protein purification. In addition, PEP also have different strains of competent *E.coli* bacteria ready for transformation, as well as various antibiotics and proteases that are commonly used in protein expression and purification. Competent cells for transformation to *Agrobacterium tumefaciens* are also available

CLONING

We offer cloning services e.g. PCR (standard cloning), subcloning, and mutagenesis.

PROTEIN EXPRESSION SYSTEMS

E. coli
Plant suspension cells

PROTEIN EXPRESSION SCREEN (SMALL SCALE)

We can run a small-scale expression test to see if your protein of interest is expressed and soluble. If you experience problems due to low solubility or low expression, we can run a small-scale experiment to test a number of different setups.

PROTEIN EXPRESSION AND PURIFICATION (SCALE UP)

We also offer scaled-up protein expression and 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.

CONTACTS (For Project request or questions regarding our services)

Mikael Lindberg, mikael.lindberg@umu.se
Uwe Sauer uwe.sauer@umu.se

MORE INFORMATION

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

Swedish Metabolomics Centre - SMC

Swedish Metabolomics Centre (SMC; www.swedishmetabolomicscentre.se) was launched in 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. Since 2016 SMC is a part of SciLifeLab. The centre aims 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).
- 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 6546 Accurate-Mass UHPLC-QTOFMSMS (2)
- Agilent 6560 Ion Mobility UHPLC-QTOFMSMS

CONTACTS

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

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

MORE INFORMATION

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

Trace Analysis Platform and Gas Isotope Ratio Mass Spectrometry - TAP and IRMS

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 and metals in complex matrices, such as environmental and biological samples. The platform supports the detection of minute quantities of analytes such as metals, organic compounds, organometallic compounds with both qualitative and quantitative methods, and gases with their isotopologues. For metals both total concentrations and speciation analysis are 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 analysis (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
- Online detection of gaseous analytes and their isotopologues

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-MS
- Gas isotope-ratio MS with direct liquid or gaseous online sampling

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: 1) Seed projects (a few samples),

2) Small projects (10s of samples) and 3) 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 mainly 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
Dmitry Shevela	Isotope-ratio MS (3:rd floor), 090-786 5293

MORE INFORMATION

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

Umeå Center 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 seven 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 Scios DualBeam is an instrument 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 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 Glacios 200 kV and Titan Krios 300 k, equipped with autoloader for cryo samples. The Cryo-EM facility was upgraded in 2022 with the Glacios and the new direct electron detectors, Falcon 4, including a new Selectris energy filter for contrast enhancement on Titan Krios. 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 BICU and UCEM provides CLEM imaging support as part of the National Microscopy Infrastructure (NMI) and offer micro-patterning on grids and cryo stage fluorescence microscopy with a Leica Thunder system. Cryo-EM facility and FIB-SEM volume imaging are SciLifeLab units. UCEM is also part of the Nordic network CryoNET organizing annual user meetings. UCEM supports sample preparation for MAX IV microscopy beamline and other synchrotron 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.

CONTACT

For general enquiries: Linda Sandblad, Facility Coordinator / Director

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

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

MORE INFORMATION

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

Technical platforms at Umeå Marine Sciences Centre - UMF

Chemical and biological analysis of marine samples

We 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.

Field projects

We also offer 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 facility

The indoor mesocosm facility includes 12 mesocosms with control of many 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.

Fish tank facility

The fish tank facility has been renovated and upgraded to allow for use of toxic substances. The temperature of three different streams of running water can be controlled. We plan to have it up for booking during 2023.

EXAMPLES OF RESEARCH

- **Temperature Fluctuation Attenuates the Effects of Warming in Estuarine Microbial Plankton Communities**, Frontiers in Marine Science, Frontiers Media S.A. 2021, Vol. 8 Marco J. Cabrerizo, *et al.*
- **An indoor pelagic mesocosm facility to simulate multiple water-column characteristics.** Int Aquat Res 10:13–29, Båmstedt U.; Larsson H. 2018.
- **Terrestrial discharges mediate trophic shifts and enhance methylmercury accumulation in estuarine biota**. Science Advances, 3(1), Jonsson, S. *et al.* 2017.
- **Differentiated availability of geochemical mercury pools controls methylmercury levels in estuarine sediment and biota.** Nature Communications, 2014 Vol.5, Jonsson, S. *et al.* 2014.
- **Increased freshwater discharge shifts the trophic balance in the coastal zone of the northern Baltic Sea**. Global Change Biology, 18(8): 2509-2519, Wikner, J., Andersson, A. 2012.

CONTACTS

Siv Huseby, Environmental analyst, siv.huseby@umu.se
Henrik Larsson, Senior research engineer, henrik.larsson@umu.se

MORE INFORMATION

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

The UPSC Microscopy Facility

The Umeå Plant Science Centre (UPSC) Microscopy Facility offers hands-on introductions, user consultation, and open-access usage following mandatory introduction based on a flat rate fee per hour for usage of equipment.

UPSC Microscopy Facility has the main focus to work with plant images and hence our confocal and multiphoton systems are tailormade for work with thick samples, have spectral detectors to adapt to autofluorescence, very sensitive HyD or GaAsP PMT detectors and long working distance objectives as well as high resolution objectives. We have sectioning equipment, motorized stages for tiling and stitching at our imaging microscopes and often both highly sensitive monochromatic cameras and color cameras. Our latest addition is a Thunder flexisystem stereo/macroscope to remove out of focus blur and thus clarify fluorescence imaging using computational clearing and adaptive deconvolution.

EQUIPMENT

- Sectioning: Cryostat – CryoStar NX70 equipped with CryoJane tape system, Vibratome VT1000S, Microtome Zeiss HM 350, Ultramicrotome – Power Tom XL
- Light microscopes: Leica DMi8 inverted fluorescence microscope, Leica 205FA epifluorescence microscope, Leica Thunder Imager Model Organism etc.
- Fluorescence Activated Cell Sorter (FACS) BD FACS Aria III Flow Cytometer
- Immunorobot: Intavis InsituPro VSI
- Atomic Force Microscope NanoWizard® 4 XP BioScience with Leica LSI HSC macroconfocal is placed on top.
- Confocal microscopes: Zeiss LSM780 CLSM with inverted stand, Zeiss LSM880 CLSM with airyscan, airyfast, PicoQuant FLIM, FLIM-FRET, FCS, FCCS and inverted stand, Zeiss LSM800 CLSM with airyscan and upright stand, Leica Stellaris 8 DIVE multiphoton with White light laser, powerful Mai-Tai multiphoton laser, Tau, Lightning and inverted stand, Nikon AZ-Z2 vertical macroconfocal

CONTACT

Facility Director:	Stephanie Robert	stephanie.robert@slu.se
Facility managers:	Marta Derba-Maceluch (light microscopes, sectioning and AFM),	marta.derba-maceluch@slu.se
	Anna Gustavsson (confocals and multiphoton)	anna.gustavsson@umu.se

MORE INFORMATION

https://www.upsc.se/platforms/microscopy-facility.html

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 two vacuum bench FTIR spectrometers, an FTIR microscope with a 64x64 focal plane array detector, two confocal Raman microscopes with 5 laser lines (from 405 to 785 nm), a fiber optic probe and polarizers, and a portable Raman spectrometer. The techniques are suitable to detect and localise (at sub/micron level) chemical changes in a wide range of samples, at high speed and low cost, non-destructively and free of external agents (dyes, markers, labels). 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 cover 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), environmental sciences and biofuel applications (from microplastics, to biochars, and algae), bio/geo/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 Licence 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 in several courses at Umeå University and SLU.

LOCATION

Chemistry Department, Building C, floors 1 and 6.

CONTACT

András Gorzsás, manager

E-mail: andras.gorzsas@umu.se

MORE INFORMATION

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

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. The new XPS spectrometer (**AXIS SUPRA+**) is under installation and expected to be in operation November 2023.

SERVICES

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 (Assoc. Prof., Dept of Chemistry), Knut Irgum (Prof., Dept of Chemistry), Jean-François Boily (Prof., Dept of Chemistry), Ludmilla Morozova-Roche (Prof., Dept of Medical Biochemistry and Biophysics)

CONTACT

Andrey Shchukarev, Dept of Chemistry, KB.C6, B6-35-07 (XPS lab) and B6-33-07 (office), tel. 090-786 5361. andrey.shchukarev@umu.se

MORE INFORMATION

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

X-Ray Diffraction Facility - XRDF

The X-Ray Diffraction Facility (XRDF) provides crystallographic expertise and access to state of the art equipment for crystal set-ups and for single crystal X-Ray Diffraction, which provides 3D structural information at atomic resolution of small molecules as well as macro-molecules such as proteins, DNA, RNA, and their complexes. X-Ray Diffraction 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®) for screening of crystallization conditions
•A Formulatrix “RockImager” for temperature controlled crystal storage and imaging and
•A “Rockmaker” liquid handling robot for screen optimization and custom screens
•A high brilliant X-Ray Diffraction system (X8 PROTEUM) with a fine focus, monochromatic X-Ray beam at $\lambda = 1.54$ Å
•A CryoStream 700 cooling system maintains the crystals at 100K during data collection
•High-end computing equipment and sophisticated software for data collection and analysis

SERVICE

•Screening for crystallization conditions
•Monitoring, evaluation and scoring of crystallization screens
•Optimization of initial screens
•Diffractions tests and iterative crystal optimization
•Full diffraction data collection incl. data processing and data analysis
•X-Ray crystal structure determination, refinement and validation
•Deposition of coordinates with the appropriate data bank, (PDB or CSD)
•Compound screens: co-crystallization with fragments and compounds (in collaboration with CBCS)
•Cryogenic preservation (vitrification) of crystals and storage in LN2

CONTACT

Uwe Sauer (coordinator):
Phone: 090-786 5930
e-mail: uwe.sauer@umu.se

MORE INFORMATION

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

Overview Infrastructure Presentations

Research Infrastructure	Contact persons	Poster	Tour
Umeå ancient DNA Lab - aDNA Lab	eric.capo@umu.se lourdes.martines.garcia@umu.se		
Biogeochemical Analytical Facility (BAF)	anders.jonsson@umu.se		
Biopolimer Analytical Platform (BAP)	junko.TS@slu.se	**P-1**	Yes
Biochemical Imaging Centre Umeå (BICU)	richard.lundmark@umu.se irene.martinez@umu.se gayathri.vegesna@umu.se	**P-3** **P-4**	Yes
BioMolecule Characterization Unit (BMCU)	ronnie.berntsson@umu.se marta.bally@umu.se johan.olofsson.edlund@umu.se	**P-8**	Yes
Computantional Analytics Support Platform (CASP)	katie.bennett@umu.se johan.trygg@umu.se	**P-17**	
Chemical Biology Consortium Sweden (CBCS)	stina.berglund.fick@umu.se erik.chorell@umu.se	**P-10**	Yes
High Performance Computing Center North (HPC2N)	info@hpc2n.umu.se pedro.ojeda-may@umu.se	**P-19**	Yes
NanoLab	roushdey.salh@umu.se	**P-16**	
National Bioinformatics Infrastructure Sweden (NBIS)	jeanette.tangrod@umu.se	**P-18**	
Nuclear Magnetic Resonance Core Facility (NMR)	mattias.hedenstrom@umu.se tobias.sparrman@umu.se jurgen.schleucher@umu.se gerhard.grobner@umu.se ilona.dudka@umu.se joao.figueira@umu.se	**P-11**	Yes
Protein Expertise Platform (PEP)	mikael.lindberg@umu.se uwe.sauer@umu.se	**P-9**	Yes
SciLifeLab site	linda.sandblad@umu.se	**P-20**	
SciLifeLab Training Hub	nina.norgren@scilifelab.se	**P-21**	
Swedish metabolomics Centre (SMC)	annika.johansson01@umu.se hans.stenlund01@umu.se swedishmetabolomicscentre@umu.se	**P-2**	Yes
Trace Analysis Platform (TAP) and Gas Isotope Ratio Mass Spectrometry (IRMS)	peter.haglund@umu.se erik.bjorn@umu.se per.liljelind@umu.se richard.lindberg@umu.se dmitry.shevela@umu.se	**P-15**	
Umeå Core Facility for Electron Microscopy (UCEM)	linda.sandbland@umu.se michael.hall@umu.se sara.henriksson@umu.se	**P-5** **P-6** **P-7**	Yes
Technical platforms at Umeå Marine Sciences Centre (UMF)	siv.huseby@umu.se henrik.larsson@umu.se annie.cox@umu.se		

Overview Infrastructure Presentations

Research Infrastructure	Contact persons	Poster	Tour
The UPSC Microscopy Facility	stephanie.robert@slu.se anna.gustavsson@umu.se marta.derba-maceluch@slu.se	**roll-up**	
Vibrational Spectroscopy Core Facility (ViSp)	andras.gorzsas@umu.se	**P-12** **P-13**	Yes
X-Ray Photoelectron Spectroscopy (XPS)	andrey.shchukarev@umu.se	**P-14**	
X-Ray Diffraction Facility (XRDF)	uwe.sauer@umu.se		

MORE INFORMATION ABOUT RESEARCH INFRASTRUCTURES AT KBC

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

PhD student presentation abstracts

Elevator talk ✓ **Poster #1**

Metabolic cooperation of bacteria within dual-species biofilms and their connection with catheter-associated urinary tract infections

Rzhepishevska Olena[1], Sokol Dmytro[1], Marinova Irina[1,2], Kladnitskiy Vitalii[1,2], Filipova Tetiana[2], Monsen Tor[1,3], Ramstedt Madeleine[1]

[1] Umeå University, Sweden
[2] Odesa I. I. Mechnikov National University, Ukraine
[3] Norrland's University Hospital, Sweden

Catheter-associated urinary tract infections (CAUTI) pose a major risk to patients, leading to serious health complications and even death. Two bacterial species, *Escherichia coli* and *Pseudomonas aeruginosa*, are commonly associated with CAUTI and are frequently found in affected patients. However, little is known about the interactions of these species forming biofilms in urethral catheters. This study aims to shed light on the metabolic relationships between these prevalent bacterial species.

We aimed to study four pairs of *E. coli* and *P. aeruginosa* previously co-isolated from patients with CAUTI. Two control strains, *E. coli* K-12 and *P. aeruginosa* PA01, were also included. Bacteria formed biofilms where they were grown in two different types of media: artificial urine medium (AUM) and Iso-Sensitest, Oxoid™ (ISO). AUM is a nutrient-limited medium, while ISO is a medium that contains glucose and amino acids/peptones. To assess the ratio of *E. coli* and *P. aeruginosa* cells within biofilms and to analyse the metabolite profiles in dual-species biofilms, the sequential culture of *E. coli* and *P. aeruginosa* in the same media (with a filtering step) to analyse the preferred type of nutrients and potential cross-feeding in the clinical pairs. The number of viable bacterial cells (VBC) of each species within biofilms was assessed using standard microbiological methods, and the biofilm metabolites were analysed by gas chromatography–mass spectrometry (GC–MS).

As a result, in ISO dual-species biofilms, *E. coli* VBC was larger than *P. aeruginosa*, while the reverse was shown in AUM. Moreover, the study showed that *E. coli* favoured glucose as a nutrient, while *P. aeruginosa* preferred organic acids. GC–MS analysis found that *E. coli* produced organic acids, like succinic acid, by metabolising glucose, which *P. aeruginosa* hypothetically consumed during sequential culturing. These results suggest that variations in bacterial metabolism can enable them to more efficiently consume nutrients found in urine, which may give them an advantage in coexisting during CAUTI.

This study highlights the importance of understanding how different bacteria work together to survive within the urinary tract. To develop better ways to treat CAUTI, we need more research to confirm these findings and explore the relationships between different bacteria.

PhD student presentation abstract

Elevator talk ✓ **Poster #2**

Unraveling mechanisms of how a gut commensal modulates Western diet-induced colonic mucus defects

Sandra Holmberg[1,2,*], Rachel Feeney[1,2,*], Vishnu Prasoodanan[1,2], Dhirendra Singh[1,2], Fabiola Puértolas-Balint[1,2], Supapit Wongkuna[1,2], Beate Brandl[3], Anni Nieminen[4], Thomas Skurk[3], Björn O. Schröder[1,2]

[1] Department of Molecular Biology, Umeå University, Sweden
[2] Laboratory for Molecular Infection Medicine Sweden (MIMS), Umeå University Sweden,
[3] Institute for Food and Health, Technical University of Munich, Germany,
[4] Institute for Molecular Medicine Finland (FIMM), University of Helsinki, Finland.
*Equal contribution

Gel-like mucus lines the epithelium of the gastrointestinal tract and serves as the first barrier against residing gut microbiota. In the distal colon, where bacterial density is highest, the constant release and expansion of mucus protects against harmful microbial interactions that could lead to inflammation and infection.

Consumption of a diet that is low in dietary fibers but high in simple sugars and fat, a so-called Western diet, leads to a microbiota-mediated reduction in mucus release and expansion ("growth") rate and increased mucus penetrability of bacteria in the distal colon of mice. While we have shown that these impairments are preventable in mice by supplementing high-fiber-driven gut microbiota, the mechanisms by which the microbiota regulate mucus function during low dietary fiber conditions and whether a similar effect is true for human microbiota are not known.

Using human-to-mouse microbiota transplantation and *ex vivo* analysis of colonic mucus function, we show that humans who increase their daily dietary fiber intake improve their gut microbiota capacity to prevent diet-mediated mucus defects in mice. We identify a responsible gut commensal that alone regulates mucus growth rate and ameliorates infection during Western diet feeding in mice. Targeted metabolomic analyses of mucus samples reveal microbial metabolites correlating with mucus function. Remarkably, upon *ex vivo* stimulation of colonic explants from Western-diet-fed mice the metabolites directly induce mucus growth. We further acquire novel mechanistic insights by identifying a downstream receptor that explains the observed phenotype.

Through our work, key players crucial for mucus function are found, increasing understanding of interactions between diet, host, and microbes. In the future, this may help to prevent mucus-associated Western diseases.

PhD student presentation abstract

Elevator talk ✓ **Poster #3**

Salvaging dNTPs for mtDNA rescue

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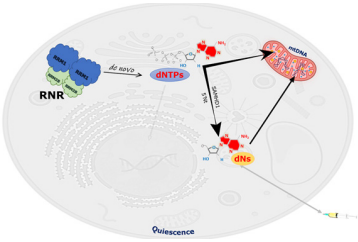

Ribonucleotide Reductases (RNRs) catalyse the committed step in de novo synthesis of deoxyribonucleoside triphosphates (dNTPs). The small subunit of mammalian RNR exists in two alternative forms: RRM2 and RRM2B. While RRM2 is found in cycling cells, RRM2B is prevalent during quiescence. Consequently, RRM2B deficiency leads to impaired synthesis of dNTPs essential for mitochondrial DNA (mtDNA) replication in quiescent cells. Unfortunately, there is presently no cure for the spectrum of mtDNA Depletion Syndromes (MDDS) associated with RRM2B mutations, ranging from neonatal lethality in autosomal recessive cases to milder, later-onset autosomal dominant forms which mainly affect sense organs.

We have developed a murine RRM2B knockout (KO) model and observed that defective de novo dNTP synthesis primarily impacts purine dNTP production; we are therefore exploiting dNTP salvage pathways for therapy. Salvage is a recycling system, whereby dNTPs are degraded into deoxynucleosides (dNs), and rephosphorylated back into dNTPs based on cellular metabolic needs. Although the precise dynamics of dN uptake and degradation in mammalian cells remain incompletely understood, our preliminary findings indicate that intravenous injection of exogenous dNs directly increases intracellular dNTP levels in various mouse organs.

SAMHD1 is a key salvage enzyme for degrading dNTPs into dNs. We have also discovered that inactivating SAMHD1 significantly elevates intracellular purine dNTP levels and extends the survival of RRM2B KO mice, albeit with a less striking impact on mtDNA copy number.

Our results demonstrate the potential for utilizing dNTP salvage pathways to ameliorate RRM2B deficiency, offering hope for patients afflicted by MDDS linked to RRM2B mutations.

PhD student presentation abstract

Elevator talk ✓ **Poster #4**

Ultra Structural Characterization of Cell Adhesion in Plants

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Cell-cell adhesion is a fundamental feature of multicellular organisms. In plants, cell-cell adhesion is mediated by the cell wall surrounding the cell. In other words, when we scale down to the cellular level, adjacent cell walls are linked to each other through a middle lamella which is believed to be very important for cell adhesion. However, it is still unclear what structural role the middle lamella plays in this process and whether other structures of the cell wall are involved. A precise characterization of cell-cell adhesion in plants is still lacking. Here, I will present our recent observations obtained using different types of electron microscopy techniques (i.e SEM and TEM). Additionally, I will also try to show how we try to combine different microscopy techniques such as fluorescence microscopy, Atomic Force Microscopy and SEM in order to gain further insight into plant cell adhesion.

Poster #5

Changes in fungal microbial community and its metabolism correspond with soil carbon accumulation in response to nitrogen addition

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Boreal forest soils are an important part of the global carbon cycle as they store a substantial portion of the soil carbon cycle, and these soils are affected by anthropogenic nitrogen deposition and fertilisation. The addition of nitrogen results in higher aboveground growth and increased above and below ground litter input. Recent studies showed that, additionally, nitrogen deposition or fertilization led to decreased soil respiration and decomposition, however, the exact mechanisms are not yet known.

We hypothesised that the reduced decomposition and respiration relate to a shift in the soil fungal community and the activity of its extracellular enzymes. Fine roots and soil samples were collected at a field site in northern Sweden, which has been fertilized yearly since 1996 with three levels of nitrogen addition (0, 12.5 or 50 kg N ha-1 yr-1). The fungal community was analysed and described using phospholipid fatty acid analysis (PLFA), ergosterol content measurements and ITS sequencing. The activities of eight extracellular enzymes connected to either nitrogen, carbon, phosphorus acquisition or oxidation were measured using colourimetric and fluorometric methods.

Based on PLFA data, nitrogen addition changed the fungal community and the abundance of both fungal and bacterial PLFAs decreased. However, ergosterol measurements showed similar fungal biomass between the nitrogen treatments. According to sequencing results, the fungal community shifted from fungi known for their nitrogen mining ability (for example Cenococcum geophilum and Cortinarius caperatus) to species without this ability (Tylospora fibrillosa and Russula griseascens). The change in the fungal community due to nitrogen addition was associated with a decrease in the activity of oxidative and nitrogen acquiring enzymes and an increase in the activity of carbon acquiring enzymes. The observed changes in soil fungal community and its activity could explain the previously observed decreased decomposition and increased carbon storage observed in the boreal forest soils after nitrogen deposition or fertilization.

Poster #6

Diet is a stronger modulator of small intestinal microbiota composition than intestinal defensins

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The intestinal microbiota is at the interface between the host and its environment and thus under constant exposure to host-derived and external modulators. While diet is considered to be an important external factor modulating microbiota composition, intestinal defensins, one of the major classes of antimicrobial peptides, have been described as key host effectors that shape the gut microbial community. However, since dietary compounds can affect defensin expression and thereby indirectly modulate the intestinal microbiota, their individual contribution on shaping gut microbiota composition remains to be defined. To disentangle the complex interaction between diet, defensins and small-intestinal microbiota we fed wild-type (WT) mice and mice lacking functionally active α-defensins (Mmp7-/- mice) either a control diet or a Western-style diet (WSD) that is rich in saturated fat and simple carbohydrates but low in dietary fiber. 16S microbiota sequencing and robust statistical analyses identified that microbiota composition was strongly affected by diet and that defensins only had a minor impact. These findings were independent of whether we compared microbiota in the lumen or at the mucosa and whether we studied the jejunum or the ileum of the two mouse genotypes. However, distinct microbial taxa were also modulated by α-defensins, which was supported by differential antimicrobial activity of ileal protein extracts. As the combination of WSD and defensin deficiency exacerbated glucose metabolism, we conclude that defensins only have a fine-tuning role in shaping the small-intestinal microbiota composition but might rather be important in protecting the host against development of diet-induced metabolic dysfunction.

Poster #7

Functional characterization of the Lysine Histidine Transporter 1 (ATLHT1)

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Balanced plant nutrition is dependent on several micro- and macronutrients and results in healthy plant growth and development. Nitrogen (N) is one of the important nutrients and its growth-promoting effects, when applied in its inorganic forms such as nitrate or ammonia, are well known. However, increased utilization of inorganic N fertilizers has negative impacts on the environment and increased the focus on organic N sources, like amino acids (AAs). AAs dominate the soil N pool of many ecosystems and different AA uptake- and transport protein families, their localization and affinities are well studied. However, the regulation mechanisms of AA transporter on a protein level are mostly unknown.

Literature has highlighted the importance of the Lysine Histidine Transporter 1 (AtLHT1) for a broad spectrum of different AAs taken up by plant roots. Here we focus on the analysis of AtLHT1, we investigate the protein-interactome of AtLHT1 in Arabidopsis thaliana, and focus on the specific interaction of AtLHT1 with a protein kinase.

This interaction suggests a posttranslational modification (PTM) of AtLHT1 in form of phosphorylation. A potential phosphorylation of AtLHT1 might serve as a fine-tuning mechanism by affecting the protein's activity. To test this hypothesis, we created AtLHT1 phospho-mutants which were screened for effects on protein activity in yeast and in plants.

We anticipate our study to be a first step towards a deeper understanding of the key AA transporter AtLHT1 and its regulation, to enable an in-depth understanding of root acquisition of organic N.

Poster #8

Structure of the reduced microsporidian proteasome bound by PI31-like peptides in dormant spores

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Proteasomes are crucial for degrading misfolded and unwanted proteins in all known eukaryotes. For intracellular pathogens with extracellular stages efficient and tightly regulated proteolysis is vital due to limited available resources. However, in microsporidia, unicellular divergent parasites with extraordinarily streamlined genomes, the proteasome complexity and structure have been unknown which hindered our understanding of how these unique pathogens adapt and compact essential eukaryotic complexes.

Here we present the cryo-electron microscopy structures of the microsporidian 20S and 26S proteasome isolated from dormant or germinated Vairimorpha necatrix spores. The discovery of PI31-like peptides, known to inhibit proteasome activity, bound simultaneously to all six active sites within the central cavity of the dormant spore proteasome, suggests reduced activity in the environmental stage. In contrast, the absence of the PI31-like peptides and the existence of 26S particles post- germination in the presence of ATP indicates that proteasomes are reactivated in nutrient-rich conditions. Structural and phylogenetic analyses reveal that microsporidian proteasomes have undergone extensive reductive evolution, lost at least two regulatory proteins, and compacted nearly every subunit.

The highly derived structure of the microsporidian proteasome, along with the minimized version of PI31 presented in this study, highlights the potential for developing specific inhibitors and provides insight into the unique evolution and biology of these medically and economically important pathogens.

Elevator talk ✓

The combination of gallium citrate with linezolid or levofloxacin enhances the inhibition of the growth of drug-resistant *Mycobacterium tuberculosis* and results alterations in the metabolome

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Gallium's inhibitory effect on Mtb growth is linked to its disruption of iron-dependent metabolic pathways in the bacterium. This disruption occurs because gallium replaces Fe3+ in enzymes but doesn't undergo the necessary redox cycling. In this study, we observed growth inhibition and alterations in the metabolome of a pre-extensively drug-resistant (pre-XDR) Mtb strain when gallium citrate was introduced into the culture medium. The primary objective was to investigate the activity of gallium in combination with relevant antibiotics against pre-XDR tuberculosis in vitro.

Aim: our aim was to compare the inhibition of growth and potential changes in the metabolome of a pre-XDR Mtb strain cultured in the presence of gallium, both alone and in combination with established anti-tuberculosis drugs.

Methods: to achieve this aim, we cultured the pre-XDR Mtb strain under different experimental conditions in triplicate. The experimental conditions included: gallium citrate alone(i), linezolid/gallium citrate (ii), levofloxacin/gallium citrate (iii), linezolid alone (iv), levofloxacin alone (v), citrate as a control to gallium citrate (vi). We then harvested Mtb cells from these cultures and subjected them to gas/liquid-chromatography mass spectrometry analysis. To understand the metabolite patterns under different conditions, we applied principal component analysis (PCA) and orthogonal partial least squares discriminant analysis (OPLS-DA).

Results: The pre-XDR-TB strain exhibited a dose-dependent response to gallium treatment, with 500uM showing greater growth inhibition compared to 250uM. Additionally, when gallium was combined with traditional antibiotics, there was an enhanced inhibition of growth. The maximum level of growth inhibition was observed in the combination of gallium and levofloxacin. Notably, different growth conditions were associated with distinct patterns of metabolites, suggesting that the combination of gallium with antibiotics led to alterations in the metabolome

PhD student presentation abstract

Elevator talk ✓

Unlock biomass potentials !

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Lignocellulosic biomass serves as a sustainable substitute for fossil resources in the production of liquid fuels, platform chemicals and other valuable commodities. The enzymatic deconstruction of biomass into sugars, which can then be converted into bio-based products presents a renewable alternative to the utilization of fossil resources. Fossil resources not only pose environmental challenges but also raise concerns related to energy security. However, it is crucial to improve bioprocessing methods efficiently to make them more competitive with fossil fuels. The key to making processes more competitive lies in achieving higher sugar yields at reduced costs.

Elevator talk ✓

Enhancing Generalization in Clustered Collaborative Learning through Objective Inconsistency

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Clustered collaborative learning trains models to address multiple individual objectives (learning tasks) in heterogeneous collaborative systems, where these objectives conflict due to the characteristics of node data. Nodes within the same clusters share similarities, while those in different clusters exhibit distinct characteristics, resulting in objective inconsistency. Recent studies have introduced various methods to enhance the performance of clustered collaborative learning. However, the primary focus is on improving the performance of individual clusters or objectives by testing with data that exhibit similar distributions. A Challenge arises when there is node data and test data distribution shift, leading to poor generalization on testing data. Therefore, improving the generalization of individual cluster models is crucial, especially given the uncertain nature of incoming test data. Fundamentally, the limited generalization capability of clusters arises from the inherent bias within the training data that is unique to each cluster. To address this challenge, we introduce a clustered collaborative approach known as Node weight Migration with Utility Enhancement Collaboration (NMUE). Leveraging the objective inconsistency between clusters, NMUE facilitates the transfer of node weights from one cluster to another, regulating the biased training weights found in the recipient clusters to enhance their utility. We evaluate NMUE across various datasets and aggregation algorithms, demonstrating its effectiveness in regularization while maintaining a favorable trade-off between personalization and generalization.

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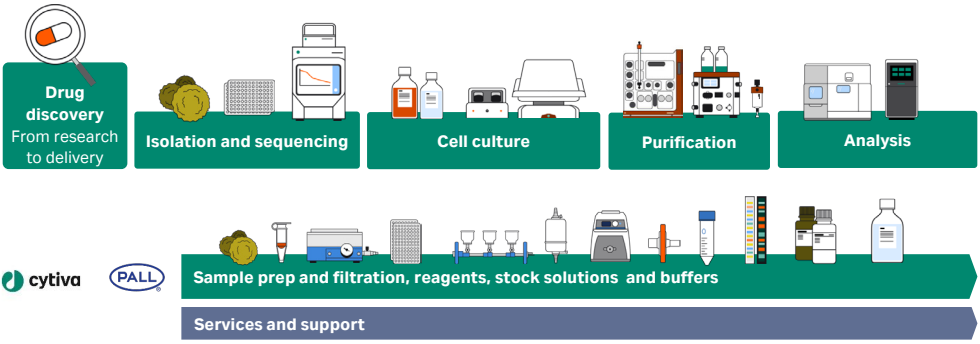

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1. Shapland EB, Holmes V, Reeves CD, et al. Low-Cost, High-throughput Sequencing of DNA Assemblies Using a Highly Multiplexed Nextera Process. Shapland et al., ACS Synth. Biol., 2015. doi.org/10.1021/sb500196n

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