XS LUND INSTITUTE OF ADVANCED NEUTRON AND X-RAY SCIENCE

Words from the Director Trevor Forsyth

Although I have only just arrived and am fresh to my new positions at LINXS and within the Lund Medical Faculty, I have in this very short time met a large number of people and participated in a number of important events that make me extremely optimistic for the future. Despite the huge problems that have arisen from the pandemic, and the fact that so many people seem to have been afflicted over the Christmas and the New Year period, there is now a general feeling that we are over the worst and finally opening up to normality.



There has been very impressive progress with the LINXS scientific

activities – both those that are reaching a conclusion as well as the second-generation themes that are starting up now - as illustrated at last year's Town Hall meeting presentations and subsequent discussions with the LINXS international Science Advisory Board (SAB). Several new themes are now developing and were presented to the Board. Liz Blackburn introduced a theme on New Materials, focusing on the development and characterisation of new materials for future applications in energy and sustainability. The Northern Lights for Food (NLF) theme has also just started, led by Selma Maric and Tommy Nylander, who have secured funding from Formas, TVV and, lately, VINNOVA. Finally, the Integrated Pharmacology and Drug Discovery (IPDD) theme initiated by Karin Lindkvist) has just started – with the core group membership including the Chief Scientific Officer and President of Pfizer, Mikael Dolsten.

It is encouraging to see that these are all of exceptionally quality, with participants from centres / groups all over Sweden and internationally. Two of them have grown out of the concluding themes – NLF from the original Imaging theme and IPDD from the Integrated Structural Biology theme, and that LINXS, as originally foreseen, is acting as an incubator for new scientific priority areas that have been identified by the scientific community. All of them are designed to make the best possible use of MAXIV and ESS as well as the other national and international infrastructures to which Sweden subscribes, emphasising the importance of interdisciplinary research, with LINXS providing a lively and collaborative environment within which themes can develop and interact with each other.

In early January, the GISANS project had its kickoff meeting and is moving ahead with its planning and preparations of the pre-study for the SAGA instrument to be built at ESS. This year's Science Day will be at the end of April and is sure to be a great event to look forward to; as you can see in the events calendar in this newsletter there are partner events, symposia and several working group meetings and hackathons in the pipeline.

I should also mention that LINXS is involved in discussions with the Project office Science Village. LINXS is of course now located in the IDEON science park but will be moving into purpose-designed premises at the Science Village Scandinavia (SVS) as soon as possible, adjacent to the MAX-IV and ESS, as plans for local, national and international engagement develop.

Please remember that LINXS supports visits from guest researchers from all over the world. The visits are aimed at supporting the LINXS mission and may have the form of short term or extended visits, discussion groups aimed at developing a collaboration or a funding initiative. If you are interested in such a visit to Lund, please contact us at info@linxs.lu.se.

Follow our progress via our website, the newsletter and social media. Please connect and re-post via LinkedIn and Twitter.



New LINXS theme launched: Integrative pharmacology and drug discovery, IPDD

LINXS is pleased to announce that the new theme Integrative pharmacology and drug discovery is launched as of January 2022 and will run for three years until end of 2024.

The IPDD theme is a very exciting development for LINXS building on the success of the previous themes and extending them to narrow the crucially important gaps that exists between molecular and cellular levels of organization, and indeed between basic scientific and clinical research. IPDD focuses on various aspects of pharmacology, from structure-based drug design of both small molecules and macromolecular drugs to their interplay with tissue and its formation, the latter with a particular focus on antibodies.

"We aim to facilitate the fundamental research within drug development via close collaboration of scientists from all the relevant topics including molecular and in vivo pharmacology, structural biology, medicinal, physical and theoretical chemistry, says **Karin Lindkvist**, theme leader and professor in Medical Structural Biology, Lund University". "Another ambition is to develop novel methods and strengthen the pharmacology community among the users of X-rays and neutrons".



The IPDD theme starting during a period of dramatic development and change in structural biology, with new approaches (e.g. protein structure prediction using AI, high-end cryo electron microscopy, neutron crystallography, enhanced throughput approaches for ligand screening and joint neutron/X-ray solution scattering analysis) are entering the mainstream alongside established approaches such as X-ray diffraction, NMR.

"The multi-technique approaches in this type of integrative effort are of central importance to the interdisciplinarity that is now essential to the optimized exploitation of the major investments Sweden has made for the MAX-IV and ESS facilities at Brunnshög as well as the international facilities to which Sweden subscribes (e.g. ILL, ISIS)", says LINXS director **Trevor Forsyth** and continues:

"It is also a driving guide for the ongoing discussions about the establishment of an Integrated Structural Biology Centre (ISBC) at Science Village (SV). This type of development has occurred at all the major X-ray and Centres (Grenoble Partnership for Structural Biology (PSB), Hamburg CSSB, PSI, RCaH) and a capability of this type at SV will be essential".

The LINXS IPDD theme will without doubt stimulate the capabilities needed to characterize a wide level of therapeutic agents and interactions and as such will be important in the development of new therapeutics. The participants in the theme and the associated working groups form a powerful grouping and include the Chief Scientific Officer of Pfizer, Mikael Dolsten. Read more at LINXS.se

Great response to 2nd Membrane Protein ws

In December 2021, the Membrane Proteins Working group held their second workshop, following up on the very successful one in May with more than 200 participants from a range of disciplines. The topics for the winter workshop was related to "Structural Resolution of Membrane Proteins: From Sample Preparation to Structural Resolution".

"The production of high-quality membrane protein crystals is always very challenging. We were able to cover many steps of the processes and get good advice on how to figure out the best way to prepare samples, which methods to use, understand more about data models and new software as well as how to conduct experiments at MAX IV, says Erika Tóth, coordinator of the workshops.



"We had really good discussions and got a broad overview of new techniques and hot topics. In this field negative results do not get published and that can lead to

that people might try to do the same things.



With this kind of open sharing, we can learn also what does not work so well. Everyone gets stuck somewhere in this pipeline", explains Erika Tóth.

The workshop offered both longer keynote presentations and smaller talks, promoting interaction and Q&A sessions. Speakers included Maria Marta Garcia Alai and Christian Löw from EMBL, Hamburg, Petra Fromme, Arizona State University, Gisela Bränden, University of Gothenburg, Allesandra Luchini, PSI and Erik Lindahl, Stockholm University.

Read more at LINXS.se

XAS school provides practical and useful skills - will be repeated annually

In the first week of November 2021, an intensive hands-on crash course in the planning, performance and evaluation of X-ray absorption spectroscopy was conducted. Inspired by the success of a long running

course, the course team, headed by Jens Uhlig, Lector at Lund University at Chemical Physics, modernised the approach and in close collaboration with MAX IV, developed a new concept.



The design consisted of one third part lectures, another third on data Analysis and the last third part on practical work, including sample preparation and a mini beamtime. The course was given by teachers from Lund university, Malmö university and MAX IV and received great interest from the very beginning.

Limited by practical aspects, much less than 50 percent of the applications could be accepted to this first round. 20 participants could join and based on an anonymous course evaluation the participants were very happy with both the concept and this

year's course and are looking forward to using their newfound skills in future work.

"Through such intensive and practical training session we are forming a new generation of scientists that can propose and perform better experiments at our facilities. This course will be repeated annually and will form the first of multiple training opportunities provided to national and international researchers by scientists under the egis of LINXS", says Jens Uhlig.

Read more at LINXS.se

A rewarding visit as a guest researcher

Professor Adam Hitchcock, McMaster University, Canada is one of the most renown and experienced researchers in x-ray adsorption microscopy and especially soft X-ray transmission microscopy (STXM). For two months in 2021 he visited Lund to support the Softimax beamline in its startup phase, educate advanced and potential synchrotron users in STXM and ptychography and to help developing methodologies, instrumentation, data and data treatment approaches.



For the LINXS community, Professor Hitchcock held a seminar in October on the subject of "Chemically sensitive imaging with synchrotron based soft X-ray STXM and ptychography". The principles of STXM and ptychography were presented, with an emphasis on spectromicroscopy. STXM, Soft X-ray scanning transmission microscopy is a powerful synchrotron-based tool for nanoscale materials analysis.

" My visit was a real pleasure. I thank LINXS and BECC at Lund University for the support of my visit. I also thank Karina Thånell and all the SoftiMax team for their friendship and great teamwork", says Adam Hitchcock.

Read more at LINXS.se

Partner opportunity: Postdoctoral fellow for joint project LU and ESS

There is a great opportunity as a postdoctoral fellow for a joint project between the Department of Chemistry, Division of Physical Chemistry, Lund University, and the European Spallation Source ERIC to investigate the mechanism of apoptosis-regulating proteins, using a combination of neutron

reflectivity and complementary techniques to probe the structure of mitochondrial membrane models reconstituted from native-like yeast lipid extracts.

The project is an international collaboration with Umeå University and the ISIS Neutron and Muon facility with a broader focus on developing experimental and analytical methodologies for mechanistic studies of membrane proteins using deuteration, neutron reflectometry and NMR.

More information about the project and how to apply for the position. Closing date: **28th February 2022**

LINXS is on Twitter

LINXS has an account on Twitter to further disseminate news and events from our institute. Please follow us there to get regular updates on our activities. Please also tag us if you want us to share news from your own organisation or to share other news on x-rays and neutrons! <u>@LINXS_Sweden</u>

We are also on LinkedIn! LINXS - Lund Institute of advanced Neutron and X-ray Science at Linkedin



LINXS events and related events

Here is a list of all the current events and activities taking place at LINXS, in partnership with LINXS or related to LINXS. Events are open to all researchers from academia and industry.

LINXS Partner Event - 18th Food Colloids Digital conference: Structure, Dynamics and Function, 10-13 April, 2022

NLF WG 2: Probing nanostructure in food and soft matter using scattering methods (Day 1 Tutorial) **25 April**, **2022**

NLF WG 2: Understanding and controlling nanostructure in food using advanced structural techniques (Day 2 Workshop aimed at Industry), **26 April, 2022**

NLF WG 3 Hackathon: Extraction of 3D structure of food from tomography images, 27-28 April, 2022

LINXS Science Day - the development and future vision of LINXS, 29 April, 2022

LINXS 3rd Integrative Structural Biology symposium in Lund, 4-6 May, 2022

Workshop Northern Lights on Food III, 1-3 June, 2022

LINXS Partner event - Lipid Bilayers at ESS- BESS in Lund, 13-15 June, 2022

LINXS Townhall meeting (and post-restriction get-together) 20 June, 2022

Northern Lights on Food 3rd Masterclass 29 August-2 September, 2022

LINXS Amyloid WG workshop: Heart, Brain and Mind, 14-15 September, 2022