



LUND
UNIVERSITY

LINXS Annual Report 2022

Contents

Executive Summary and reflections from the LINXS Director	2
1. The mission of LINXS	4
2. Reflections from the Scientific Advisory Board	4
3. LINXS scientific achievements and impact	4
3.1. New Materials Theme summary of outcomes and reflections	5
3.2. Northern Lights on Food (NLF) Theme summary of outcomes and reflections.....	6
3.3. Integrative Pharmacology and Drug Discovery (IPDD) Theme summary of outcomes and reflections	8
3.4. Final Integrative Structural Biology (ISB) Theme summary of outcomes and reflections.....	10
3.5. SAGA-Preparing for a GISANS instrument at ESS – A Swedish Initiative	12
3.6. LMK Post-doctoral fellow in transthyretin (TTR) amyloidosis.....	13
3.7. CoWork summary of outcomes and impact potential	13
4. LINXS Strategic & Operational Achievements.....	14
4.1. Communications as a pathway to impact.....	21
5. LINXS in numbers 2022.....	23
6. Annual Financial Report 2022.....	27
Annex 1 – LINXS Themes and Working Groups in 2022	28
Annex 2 – List of LINXS activities 2022	30
Annex 3 – List of publications with LINXS affiliation 2022	33
Annex 4 – LINXS Community 2022.....	40
Annex 5 – Financial reporting 2022	42
Annex 6 – Highlights and Legacy 2022.....	44
Highlights – New Materials Theme.....	44
Highlights – Northern Lights on Food Theme (NLF)	45
Highlights – Integrative Pharmacology and Drug Discovery Theme (IPDD).....	49
Legacy statement – Integrative Structural Biology Theme (ISB)	52
Highlights - Collaboration	55

Executive Summary and reflections from the LINXS Director

2022 has been a remarkable year for everyone, and certainly a remarkable one for LINXS as a developing institute. The passing of the pandemic and turbulent world affairs has left conflicting feelings of recovery, uncertainty, and opportunity – with pervasive sense of unpredictability and urgency. During this period, LINXS has grown with increasing confidence in its mission for Sweden as well as for the large-scale infrastructures and the international landscape. A great deal of this progress has been due to the previous LINXS managements: Peter Schurtenberger as the original director brought LINXS into existence as an advanced study institute, and Stephen Hall maintained and developed it throughout the very challenging circumstances of the pandemic. Increased digital and hybrid engagement is now part of our daily lives and has helped establish LINXS as a physical and digital platform of wide international transdisciplinary scientific interaction – as well as minimising unnecessary travel.

As many of you will know, LINXS' core activities are based around fixed-length scientific Themes that are proposed competitively by the scientific community and reviewed by an independent external Scientific Advisory Board (SAB). Themes typically fall into science areas that can be addressed using techniques often related to areas of hard condensed matter, soft condensed matter, and life sciences research – although the Themes themselves may not be confined by these areas. During early 2022, a new Theme entitled Integrative Pharmacology and Drug Discovery (IPDD) started its activities, with working groups focused on pharmacology, with activities covering structure-based drug design, macromolecular drugs/antibodies, biomedical imaging, and drug delivery. The IPDD core group contains the Chief Scientific Advisor of Pfizer (Mikael Dolsten). It joins the existing Themes on New Materials, and Northern Lights on Food, which have also been very active during 2022.

We were also very pleased to host several schools: continuing the very successful CoWork webinar series dedicated to the exploitation of the coherence properties of X-rays and initiating the IPDD Antibodies in Solution LINXS-NIST webinar series designed as an educational venture into antibody research using scattering methods. During the year it was good to see guest researchers returning to LINXS and that the interest is growing rapidly.

It is important to emphasise that LINXS activities contribute to an extensive repository of educational material. Webinars and recorded presentations are continuously accumulating, and work on structuring and customising this resource to meet the various levels of scientific need accessibility is ongoing. This repository grew significantly during the year to 130+ items - and is still growing rapidly. Numerous consortia created via the LINXS Themes have procured substantial funding and facility beam time allocations. Scientists involved in the Northern Lights on Food Theme have been funded by VR for a national project focused on a GSANS instrument at ESS (SAGA GSANS). Generous funding from the LMK Foundation has also been obtained for research on the molecular work relating to amyloidosis. The postdoctoral researchers associated with both these projects - Sebastian Köhler and Daniel Sarabi respectively - contribute to day-day activities at LINXS and help develop connectivity with early-stage researchers.

Throughout the year, LINXS has been building an increasingly open agenda with the Swedish scientific community as well a deepening engagement with the international communities. The model for LINXS Theme applications has been developed in a way that now allows principal

investigators to apply from anywhere, greatly broadening the scientific scope and volume of LINXS activities. This led to the first open (international) Theme call autumn 2022. These will be reviewed by the LINXS SAB as part of a two-stage application process, with outcomes announced in spring 2023, and successful Themes starting the following September. This will result in substantial growth of LINXS Thematic activities and scientific engagement. In parallel with this, LINXS has also (in collaboration with MAX IV and ESS) applied to the Swedish Research Council for the creation of a LINXS Centre of Excellence. A successful outcome to this proposal will provide funding for LINXS Themes led by scientists/groups from anywhere Sweden, extending the resourcing of its mission to develop interdisciplinary science over the country. In addition, LINXS also intends to apply for MSCA COFUND resourcing from the European Commission to fund over 40 postdoctoral researchers for a project entitled Advanced Multiscale Biological Imaging using European Research Infrastructures (AMBER). This project will be designed to empower a wide range of European scientific capability ranging from clinical imaging through to molecular characterization, bridging length scale and inter-sectoral science gaps and making crucial impact on the need to develop the principal investigator user base of the future.

2022 has also been an extremely important year in terms of the LINXS arrangements to move onto the Science Village in the short/medium term - a move that will place us right in the middle of a brand new national and international science environment in close physical proximity to both the MAX IV and ESS. The LINXS Board is evaluating attractive bids that were made by different companies at its latest meeting – these will be discussed in detail during 2023.

We are deeply grateful to many people for the success of this year. The LINXS SAB has of course played a crucial role in helping us chart the way forward and I would like to say a special thanks to Stefan Egelhaaf (SAB Chairperson, currently on leave for personal reasons) for the huge contribution he has made, and to Christiane Alba-Simionesco for stepping in at short notice). We are also very grateful to our Board members and to Anders Tunlid who as the Chair has played a vital role in providing constructive guidance during a time of substantial change and development.

On a more personal note, I would like to thank the other members of the LINXS management team (Marie Skepö, Oxana Klementieva, Jörgen Larsson, Anna Niinidou) for their unfailing contributions – with a particular word to Anna given the tower of strength she has been to us despite her own period of great adversity. A special thanks also to Stephen Hall for taking the time to overlap with me during my first 6 months as Director, to Martin Stankovski for the huge amount of strategic advice he has provided as well as enormous contributions to numerous application processes, and to Noomi Egan to the large effort she has put into outreach activity, including the Newsletter. We will miss Åsa Grunning who left for another assignment during the year. Åsa had been with LINXS since the start and had a very strong impact. However, we were very lucky to have had the help of Nina Ahlbeck and Marianne Loor during this period. We are currently in the process of defining a position to replace Åsa as activities coordinator. Most importantly I would like to thank you – our scientific community – for the drive and enthusiasm that is the main reason for our existence and indeed that of the infrastructures developing around us!

Trevor Forsyth,
LINXS Director

1. The mission of LINXS

Establish LINXS as a world leading advanced study institute for all scientific and technological disciplines which can benefit from the use of neutrons and X-rays.

Attract outstanding scientists for short-term focused research visits to contribute to excellent science. The goal is to further research collaboration within national and international research networks, especially for early career researchers.

Promote science and education focusing on use of neutrons and X-rays in research and development, and help educate potential users of ESS, MAX IV and other major research infrastructures to enable ground-breaking research.

Create international networks and enhance the visibility of Sweden internationally in the use of neutrons and X-rays. We want to invigorate the dialogue between academia and society in all aspects of large-scale research infrastructures using neutrons and X-rays. The goal is to become a nucleus for local, national, and international activities in Science Village Scandinavia and a think-tank initiating new ideas and themes.

2. Reflections from the Scientific Advisory Board

The LINXS Scientific Advisory Board (SAB) is made up of high-level international researchers in science involving neutrons and x-rays. The SAB provides advice on the scientific direction and strategy for LINXS, including reviewing applications for new Themes. The SAB provided the following summary of their impressions on the LINXS scientific activities in 2022.

“The SAB members would like to express our sincere gratitude and support to Professor Stefan Egelhaaf, chair of the SAB until the fall, and our best wishes. The SAB is very happy to welcome two new members Annette Langkilde and Alexandra Pacureanu, both specialists in the focus area of Life Sciences.

LINXS long-term scientific strategy - The SAB would like to congratulate the LINXS management on the recent progress it has made and for the dynamism of the Institute. LINXS has clearly passed to a new stage in its development with:

- a greater national visibility with a corresponding update of the name,
- the first international call for Themes, and
- a project for a LINXS Centre of Excellence, with a VR proposal that will expand LINXS capacity to 8 Themes instead of the current 3.

With the last expansion, LINXS would be able to access a national rather than local coordination role between universities, industries, and institutes, ensuring independent funding. The SAB strongly supports and welcomes all these actions.”

3. LINXS scientific achievements and impact

In 2022 there were three Themes active, and one in the process of concluding after the inevitable delays caused by the pandemic. The recent Theme “Northern Lights on Food” was ramping up its activities with 5 working groups starting up in the period, and “New Materials” was hitting its stride, also with 5 working groups active. “Integrative Structural

Biology”, with its 6 working groups, concluded in 2022 with some final activities. The new Theme “commenced in 2022 and ramped up activities.

3.1. New Materials Theme summary of outcomes and reflections

The New Materials for Energy and Sustainability Theme pushes forward the development and characterization of new materials with potential future applications in the fields of energy and sustainability, bringing together X-ray and neutron experts with material development experts. The Theme was in its second year in 2022 and the individual working groups started developing very clear and distinct identities. Each working group has ended up focusing on particular aspects of the overall LINXS mission. As an ensemble, the Theme has been active in teaching the next generation of experts, via specialist schools and training sessions, developing data analysis methods and tools for both the expert and the newcomer, and in developing networks laserling in on key scientific questions.

The Theme started during the Covid era, and it was still feeling the effects in 2022 on many of its activities. One key issue has been the difficulty in inviting visiting researchers to LINXS to participate in shared activities. Previously, the Theme’s only visitor had been Prof. Regina Dittmann (FZ Jülich and RWTH Aachen) which visited as a part of the Nanostructures and Interfaces Working Group’s activities. After that visit, she was nominated independently for a Lise Meitner professorship in 2022 at Lund University. In 2022, the Theme’s first long-term visitor was Prof. Jason Weaver (University of Florida, US), who was hosted by the Catalysis working group over the summer. He took part in several of their activities and gave several seminars at different institutions. The visiting fellow programme is ramping up in 2023 as the prospects for travel have become more reliable.

The Working Groups have put in a coordinated effort to promote in-person meetings, supplemented with hybrid accessibility. A key example here is the series of workshops on catalysis organised by the Catalysis Working Group. This has brought together a number of distinguished researchers, primarily from around Europe, but using the Visiting Fellow programme to ensure contact with the US community via Prof. Weaver.

The Functional Magnetic Materials Working Group also brought together researchers in the magnetic small angle neutron scattering community from around the world to develop a priority list on how to improve the data analysis workflow, both for standard experiments and for more unusual ones. This is in direct response to the workshops held previously by this working group in 2021, that had identified this issue as a particular bottleneck, in particular to more widespread adoption of small angle neutron studies on magnetic materials. Participants included both long-standing experts and new doctoral students. The Working Group was able to engage scientists involved in a well-established open-source analysis program, SasView, that is well supported by the community. Following directly on from the working group’s workshop, there was a SasView CodeCamp, involving some of the LINXS participants, to start to put the plan into action. Following up on this is a scheduled activity for 2023.

Of course, there were also some problems. In 2021, the Charge Transfer Materials and Light Harvesting Processes Working Group had run a successful school for hands-on training in the design, performance, and analysis of X-ray Absorption Spectroscopy experiments. A key component of this was the coupling with experimental time at the BALDER beamline at MAX-IV. The second edition of the school could not take place in autumn 2022 as planned,

as it was not possible to schedule the beamtime at BALDER at the right time, but the school has been scheduled to take place in March 2023. The working group's ambition is to develop this into a sustainable long-term activity after the end of the Theme.

Finally, the Nanostructures and Interfaces working group planned activities which did not materialise in 2022, but actively participated and contributed in a fruitful way in activities of other working groups within the Theme.

New Materials Theme highlights can be found in Annex 6.

3.2. Northern Lights on Food (NLF) Theme summary of outcomes and reflections

The Northern Lights on Food (NLF) Theme was started to bring together expertise in food science and technology together with experts in characterization methods using neutrons and X-rays as well as other complementary techniques to generate new knowledge and cutting-edge technology within food science. The aim is to advance food science by bringing together complementary expertise within the area, not only to take full advantage of the research tools provided by ESS and MAX IV, but also to provide a wider societal impact.

The Theme took active part in the 18th Food colloids digital conference: Structure, Dynamics and Function, Apr 10-13, 2022.

Northern Lights on Food III was the third annual conference bringing together 80 researchers from academia and industry and was held at Palaestra in Lund June 1-3, 2022. Three days of presentations included new research using X-ray and neutron tools to make progress in our understanding of food structures, as well as connections to the wider food industry and society as a whole.

Northern Lights on Food together with Business Sweden hosted a delegation from San Francisco area 5 June 2022. 20 people with an interest in food, including entrepreneurs, investors, those in food tech, and chefs, spent a day in Lund to learn more about the latest food research at Lund University, and within Northern Lights on Food, as well as to start new collaborations.

Northern Lights on Food held a breakfast event as part of the Skåne Innovation Week on the 16th of June with food scientists working in the research environment around MAX IV and ESS. The platform was presented by Tommy Nylander, and researchers displayed posters about designing future foods.

The 3rd Northern Lights on Food Masterclass was held 29 August -2 September 2022 with 30 participants and hands-on exercises at Copenhagen University. The theme of the Masterclass was how X-ray and neutron scattering can reveal the complexity of food materials.

A Vinnova sponsored project, "Strengthened research and innovation in the food sector made possible by neutron and synchrotron technologies" aimed to increase the participation of senior scientists in the food sector in the LINXS Northern Lights on Food Theme, held a meeting at ESS and LINXS 17-18 October 2022. Scientists from RISE, Örebro University, Linné University, SLU, KTH, Chalmers, and Livsmedelsföretagen participated.

A Joint LINXS/ Physical Chemistry/ KILU/ Food Technology, Engineering and Nutrition seminar, "Processing-Structure-Property Relationships of Plant-Based Protein Products" was given by Dr Leonie van 't Hag, Monash University, Melbourne, Australia.

Apart from the above-mentioned Theme activities the 5 working Groups organised the following events in 2022:

WG 1 - Structure of Food Raw Materials: Focus on the relationship between the structures of raw materials and process conditions. (Nick Sirijovski, Oatly; Maud Langton, SLU; Francesco Vilaplana, KTH). Hackathon was jointly with WG 3.

WG 2 - Food Colloids: Focus on the colloidal and interfacial phenomena to build up the complex food matrix. (Ben Boyd, Copenhagen Uni; Jacob Kirkensgaard, Copenhagen Uni): A food Colloids and Structured Interfaces Industry Workshop was held as a hybrid meeting on Oct 4, 2022.

WG 3 - Structure of Food during Processing: (Stephen Hall, LU; Niklas Lorén, RISE): A Northern Lights on Food 3D imaging hackathon was held Apr 27-28, 2022. This also involved WG1.

WG 4 - Food Interactions on Surfaces: Focus on the interface between food and processing surfaces, attachments of microorganisms, as well as food and packaging materials. (Tommy Nylander, LU; Jenny Schelin, LU; Martin Adell, Tetra Pak): A first meeting for the year was held on Mar 18, 2022. A follow up workshop was held on May 11, 2022.

WG 5 - Food and health: (Peter Spéjel, LU; Greg Smith, ISIS; Anna Ström, Chalmers): A webinar on the study of lipid structures in membranes and food formulations was held on Feb 8, 2022. Dr Marta Martinez-Sanz, Institute of Food Science Research (CIAL-CSIC), Spain gave a webinar, "Scattering techniques to investigate the nanostructure and digestion mechanism of polysaccharide-based emulsion gels" together with Prof. Judith Peters, Université Grenoble Alpes, Grenoble, France "Dynamics of Apolipoprotein B-100, the moiety of low-density lipoproteins" on Nov 11, 2022.

Northern Lights on Food Visiting Fellows

LINXS Visiting Fellow Prof Elliot Gilbert, Food Materials Science, Australian Nuclear Science and Technology Organisation (ANSTO) took a very active part in the Northern Lights on Food activities June-July 2022. In particular, he helped formulate the strategy for creating a European Food Laboratory. LINXS guest professor Jeremy Lakey, Structural Biochemistry, Biosciences Institute, Newcastle University, UK, led a discussion session on Jun 9, 2022.

Funding initiatives

The Northern Lights on Food Lund members applied to become a Lund University profile area. The proposal was not selected among the 5 granted but were favourably judged and got 600 000 SEK to strengthen the case. A new call is expected during 2023.

Niklas Lorén (RISE), Judith Houston (ESS), Roland Kádár (Chalmers), Tommy Nylander (Lund University), Mats Stading (RISE), Ann Terry (MAX IV) submitted an infrastructure proposal

“Extruder for in situ structure characterisation of sustainable protein melts using photons and neutrons” to Swedish Research Council – VR. Decision pending.

A pitch to the Novo Nordisk Foundation for “An International Center for Advanced Food Structure Studies” was made together with Copenhagen and Aarhus Universities on the 14th of December 2022. The pitch was very well received, and NLF will be invited to another meeting in the beginning of 2023.

Funding obtained for Northern Lights on Food Activities: (in operation from past years)

- Northern Lights on Food - knowledge and innovation for a green transition in the food sector. (Grant ID: 20307448, Swedish Agency for Economic and Regional Growth, EU European Regional Development Fund and Skåne Region). This is complementary to the NLF Theme as it provides means to conduct smaller key research projects within all the 5 working group areas to demonstrate the large impact structural studies using X-rays and neutrons can have.
- European Food Laboratory (EuFL) – Case study. (The research and innovation council of Skåne (FIRS)). The main activity is to build the case for a long-term funding of Northern Lights on Food. During 2022 a Novo Nordisk Foundation has been approached and the initiative was well received.
- Strengthen food sector research and innovation by enabling use of neutron and synchrotron techniques. (2021-04909, Vinnova). This funding was obtained to open up the NLF LINXS activities to all Swedish universities with activities in the food sector to take an active part and to engage their colleagues at their home universities. For this purpose, each partner was provided with funding corresponding to the salary contribution to LU-LINXS fellows.

Northern Lights on Food (NLF) Theme highlights can be found in Annex 6.

3.3. Integrative Pharmacology and Drug Discovery (IPDD) Theme summary of outcomes and reflections

2022 was a successful year for the Integrative Pharmacology and Drug Discovery (IPDD) Theme, and its first year as a LINXS Theme. IPDD includes three working groups, the Structure-based drug design, the Macromolecular Drugs-Antibodies and the Biomedical Imaging. The Theme focuses on various aspects of pharmacology, going from structure-based drug design of both small molecules and macromolecular drugs to their interplay with tissue and its formulation. During 2022 the Theme has had several activities within the different working groups (described in detail below) but also a very successful kick-off for the whole Theme. The kick-off took place in May and gathered around 50 participants at LINXS premises. The different working groups gave presentations, and there was also a successful round-table discussion session to plan for the upcoming events. The IPDD core group (including the working groups leaders) meet every second week (online) and discuss the work that is going on within the working groups and at LINXS. In addition, the core group gave a seminar at NextBioForm, which was very well received.

The **Structure based drug design (SBDD)** working group consists of 14 members from different disciplines within the SBDD topics working at Lund University, as well as other universities or research facilities in Sweden and two members from abroad. The group had its first meeting on zoom in March 2022 where the members could introduce themselves and

discuss the upcoming activities. During the year they kept active contact via e-mail and zoom meetings. The main goal for the 2022 was to organize a lunch-to-lunch scientific meeting on SBDD topic. This meeting has been successfully held on November 14-15th, 2022. The meeting took place at LINXS premises and around 40 participants from all over Sweden and also a few from abroad joined the event. Several keynote speakers from both academia and industry as well as participants presented their research of high scientific quality covering various aspects of SBDD. Also, there was a poster session, which was especially appreciated by the students who were happy to present and discuss their work.

Due to the success of the meeting the working group plans to organize a similar event in 2023. By the end of 2022 the working group also started a discussion and prepared a first draft for the major planned event in 2023 – a course on Fragment base lead discovery.

The **Macromolecular Drugs-Antibodies** working group continued its “Antibodies in Solution research programme” in 2022. This research programme has the aim to increase knowledge on the properties of individual antibodies as well as those of concentrated solutions and gathers 14 international research groups, the American National Institute of Standards and Technology (NIST), and the pharmaceutical company Novartis in Switzerland.

Throughout the entire year of 2022 and in parallel to the ongoing X-ray, neutron and complementary experiments, the members of the individual Work Packages of the research programme have had regular Zoom meetings, always in close collaboration and vivid exchange with interested NIST scientists. The Antibodies in Solution research programme had a successful [mid-term meeting in September 2022](#). The aim was to discuss the experimental and simulation results that the individual consortium members had collected so far on the NIST antibody (NISTmAb) and tackle important scientific questions. Representatives from the 14 research groups, the American National Institute of Standards and Technology (NIST), and the pharmaceutical company Novartis joined the meeting in Lund. One of the important outcomes of the meeting was that in addition to the NISTmAb, a new antibody will be provided by Novartis free of charge.

In a nutshell, the Research Programme has achieved the following results within 2022:

- Performed an extensive screening of solution conditions, characterized the resulting overall protein interactions, and subsequently defined the experimental conditions and the preparation protocol for the first of several planned model systems.
- Demonstrated the existence of isotope effects when working with either normal or heavy water-based solvents required by some of the relevant techniques used by the consortium.
- The collaboration between the theory/simulation groups and the teams from the experimental work packages has led to the development of so-called coarse-graining strategies for the analysis of experimental data and first successful applications of such models in order to understand the resulting solution properties and in particular treat charge effects in mAb solutions.
- The research programme was identified as an important research effort by Novartis, who agreed to join under the same conditions (open research collaboration) and provide the consortium with a second model mAb with different properties, thus further increasing the future impact of the research programme.

In the end of 2022, the Macromolecular Drugs-Antibodies working group launched the [Antibodies in solution: A LINXS-NIST Webinar Series](#).

This Webinar Series is meant as an educational venture addressed to a broad audience including students and researchers from various backgrounds and all those who are interested to dive into the fascinating world of antibody research and learn more about the use of scattering methods for this purpose.

The **Biomedical Imaging** working group was founded during spring 2022. It has eleven active members representing both academy and industry including members from Denmark and France. The group meet regularly every two weeks for which there are written minutes. The group co-organized a LINXS imaging workshop May 11th, "Imaging possibilities for breakthrough in medical research". Lars E. Olsson also gave an introductory talk.

A dedicated LINXS workshop on "Biomedical Imaging for drug discovery/development – Opportunities for MAX IV" was organized in October 2022. It had 40 participants on-site and another 20 on-line. During the workshop, scientists from the pharmaceutical industry explained the process and the hurdles in drug discovery and development, and how biomedical imaging can be used to facilitate the process. Educational lectures were also given, which reviewed the imaging methods for both synchrotron imaging and competing imaging technologies. In addition, state-of-the-art lectures on biomedical imaging applications from the synchrotron facilities at ESRF and PSI, were also presented. During December a dialog with the Life science director Marjolein Thunnissen was commenced. Several different initiatives and funding applications were outlined that would facilitate the MedMAX beamline. These will be on the to-do-list for 2023. At the end of the year Lars E. Olsson resigned as group leader and from 2023 Martin Bech is the new group leader.

During 2022 IPDD also initiated the discussions to start a new working group focusing on Drug Delivery. Dr Vito Foderà at Copenhagen University at the Department of Pharmacy will lead the working group that will be started in Jan 2023.

Integrative Pharmacology and Drug Discovery (IPDD) Theme highlights can be found in Annex 6.

3.4. Final Integrative Structural Biology (ISB) Theme summary of outcomes and reflections

2021 was the last year for the Integrative Structural Biology Theme, but since the big showstopper - the COVID-19 pandemic, had affected many of the planned activities, ISB had events also during 2022. After two very successful ISB symposia in 2018 and 2019, the ISB core group decided to have the final ISB symposium the 4-6th of May in 2022. The final meeting, with approximately 100 participants, was truly successful. The three days meeting was inspiring, with the program having a mix of invited keynote speakers as well as many short talks which created a lot of interactions. In addition, there was a round table discussion centred around the future for structural biology, which was very well received. The discussions were centred around how structural biology can be better intertwined with the clinics, and how structural biology can contribute even more in the future and how the communication can be improved.

The Theme definitely contributed to a stronger and better communication between scientific areas that was previously more separated. Although ISB has come to an end within LINXS, the Theme has contributed to many important things for structural biology in Sweden and the Nordic countries. This is supported by the fact that ScilifeLab initiated an ISB platform in 2021 (<https://www.scilifelab.se/news/infrastructure-update-the-integrated-structural-biology-platform-isb/>) showing the importance of integrative research within the structural biology community in Sweden. In addition, an application to the NordForsk foundation to continue strong collaborations within integrative structural biology in the Nordic countries was submitted in the end of 2022.

Another initiative to strengthen ISB research in Lund was the start of the working group, **Lund Integrative Structural Biology Centre Initiative (ISBC)** in 2020. The aim of the working group was to investigate if there is an interest, in the Lund area, of a future integrative structural biology centre placed at Brunshög, and to help catalysing the discussion and development of these ideas. A workshop was held in February 2021, four invited speakers from integrative structural biology centres in Europe. For this meeting, PIs that are directly working with structural biology in the Lund were invited. After the meeting the participants were asked to fill in a survey. One question was if the invited PIs thought that an ISB centre should be established in Lund, and 93% of the participants were positive towards the establishment of ISBC. As such a positive response was received, the working group decided to go further with the plans and submitted a letter to the University management. The letter was also received very well from the management and currently there are ongoing discussion on how this will be funded.

During 2022 the working group worked intensely towards that Integrative structural biology would become a scientific profile area at LU. It was well received, and was selected for interview, but was unfortunately not selected as one of the five profile areas in the end.

The **Membrane Protein** working group was formed towards the end of 2019 after a couple of brainstorming meetings with both local and international participants interested in the research area. The outcome of these meetings was the successful official formation of the Working group, identification key topics that will be addressed and suggestions for activities. During 2021, the group has had two successful workshops, the first focusing on protein expression and sample quality control; and the second focused on sample preparation for structural biology and structure determination by different methods such as X-ray crystallography, neutron crystallography and single-particle cryo-EM. Both workshops were held online with roughly 100 participants from all over the world.

The **Amyloid** working group organized a workshop focused on "User-friendly analysis of spectroscopy data with Quasar - multivariate statistics and machine learning" which occurred as an online event in May and resulted in a follow up workshop on January 22nd. This activity was based on a collaboration between the French SOLEIL light source, MAX IV and the Faculty of Medicine. A meeting entitled "Heart and Mind", focusing on the cardiomyopathy and neuropathy in relation to amyloidogenesis was held on March 5th, 2021.

As a follow up activity the group produced a conference report published in Journal of Translational Medicine: "Recommendations for addressing the translational gap between experimental and clinical research on amyloid diseases This paper is a report of recommendations for addressing translational challenges in amyloid disease research."

prepared by the group members. The key suggestions include improving cross-cultural communication between basic science and clinical research, increasing the influence of scientific societies and journals (vis-à-vis funding agencies and pharmaceutical companies), improving the dissemination of negative results, and strengthening the ethos of science. DOI: 10.1186/s12967-022-03420-9.

Members of the amyloid group have also been involved in outreach activities, delivering seminars and teaching. For example, Dr Oxana Klementieva, a senior lecturer at LU medical faculty and LINXS co-Director, delivered a lecture at SciLifeLab entitled “How to become a Life Science researcher that uses synchrotron light and neutron applications” in September, and has also been involved in a PhD course on “MAX IV/ESS-based imaging for medical and biomedical research”.

The **Time-resolved Structural Biology** working group has during 2022 concentrated on the organisation of the second Time-Resolved Structural Biology workshop, which was held at LINXS on October 26th-28th as an in-person meeting. While the first workshop had a broad programme that highlighted what can be done with different methods, the second workshop focused more on crystallography, including experiment design, results and facilities, and also more talks and discussions on data interpretation, how to avoid pitfalls, and on what developments that are important for the field. In terms of techniques the programme covered NMR, SAXS, CryoEM crystallography, and computational methods. The workshop was held Wednesday-Friday lunch-to-lunch at LINXS but with Thursday afternoon at the MAX IV Laboratory including a visit of the facility and the new MicroMAX beamline. In addition to a longer discussion session for each half day, the coffee breaks, lunches, poster session and the workshop dinner on Thursday evening gave ample of time for interaction between the workshop participants. This contributed to the positive feedback received, and hopefully another workshop in this series can be organized two years after the second one. The workshop had 48 participants including 18 speakers (plus one remote speaker) and a discussion moderator.

Integrative Structural Biology (ISB) Theme closing event and legacy statement can be found in Annex 6.

3.5. SAGA-Preparing for a GISANS instrument at ESS – A Swedish Initiative

Swedish universities, institutes and companies collaborate on planning new instruments for installation at ESS, the world's most powerful research facility for neutron radiation, outside Lund. A dedicated Grazing-Incidence Small-Angle Neutron Scattering (GISANS) instrument will enable researchers to analyse in detail how a neutron beam spreads when reflected from a surface. Here LINXS has served as a meeting point and a hub to solidify the collaboration. The Swedish Research Council in November granted funding (2021-06230) for an interdisciplinary project “Preparing for a GISANS instrument at ESS – A Swedish Initiative” with Tommy Nylander as project leader. This project, SAGA, are jointly conducted by Lund University, Uppsala University, Malmö University, Linköping University and KTH. A Postdoctoral fellow, Sebastian Köhler, was hired for 3 years during 2022 and placed at LINXS. He has started the design work on a potential instrument in close collaboration with ESS and the project partners. A kick-off the SAGA was held on Jan 14, 2022. This was followed up with a SAGA GISANS workshop was held on 12 of May in connection with the

Swedish Neutron week 10-12 of May in Kolmården, outside Linköping. Professor Regine von Klitzing, University of Darmstadt, was invited as a key-note speaker. A Saga Gisans update meeting was held in connection to MAX IV & ESS user meetings on Oct 4, 2022. Apart from update of the project, there was also an invited talk from Dr. Sarah Rogers, ISIS, STFC-Rutherford Laboratory, UK and Henrich Frielinghaus, Jülich Centre for Neutron Scattering, Garching, Germany. An update of the SAGA sister project, HIBEAM- A fundamental physics beamline for ESS, was given by Dr Valentina Santoro, ESS. The funding agency, Swedish Research Council, was well represented by Johan Holmberg, Niklas Ottosson and Maja Hellsing.

3.6. LMK Post-doctoral fellow in transthyretin (TTR) amyloidosis

Dr Daniel Sarabi, the LINXS LMK Post-doctoral researcher supervised by Trevor Forsyth was hired in June 2022 with funding obtained by the LMK Foundation to work on in transthyretin (TTR) amyloidosis.

During the year, Daniel has obtained access to a high-performance computing cluster (HPC) LUNARC, Aurora in Lund University via Prof Marie Skepö, head of the division for theoretical chemistry. He is running molecular dynamics simulations on the tetrameric structure wild-type and two mutants, in order to estimate the change in protein stability upon amino acid mutation. This work is based on the previous work led by Professor Trevor Forsyth, and therefore, the first objective which is ongoing now, is to replicate the results achieved previously, prior to exploring mutants and alchemical perturbations on the tetramer, dimer, and monomeric structures of TTR. Thus, building up the system, utilizing the correct software tools, and writing scripts that allows us to build up a pipeline for running these simulations is the ongoing work that will allow us to analyse the effect of mutations on TTR stability.

Daniel initiated the following LINXS activities:

- Created a young research science symposium for life science initiative, which will take place on the 13th of March 2023. The aim is to bring together young researchers (PhD and Postdocs) nationally and internationally that utilize X-rays and neutrons from a wide variety of research fields and applications, in order to create opportunities for collaboration and networking. This would hopefully lead to new and exciting projects that would directly increase the usage of facilities such as MAX IV and ESS.
- Together with LINXS employee Dr Martin Stankovski and LINXS PhD board representative Sandra Benter, reorganizing and restructuring the educational material on the LINXS website. This work is intended to increase the usability of our educational material regarding X-ray and neutron science for students and researchers.
- Contributed to the increase of the education materials platform and LINXS YouTube channel through processing recorded material.
- Contributed to different LINXS activities such as workshops, courses, seminars, conferences, and Theme related events.

3.7. CoWork summary of outcomes and impact potential

CoWork is a webinar series mutated from a “Coherence Workshop”, originally planned for October 2020 and cancelled due to the world pandemic. Initiated and driven by Gerardina (Dina) Carbone, MAX IV Laboratory, this series has been followed with interest since its beginning and is continuing without interruption until today. 32 renown scientists worldwide have already contributed to this series until the end of 2022. Five webinars are already

planned for 2023 and more will be scheduled on an ongoing basis. As a side note, only one scientist has never replied to attempts to contact them as a potential speaker. Everyone else has accepted the invitation with enthusiasm.

The attendees are from a wide international community of experts and of newbies (many from European countries, USA, and Brazil and a few from Canada, India, Taiwan, and Australia). Their number has increased by a factor of ten since the beginning of the series, reaching an impressive count of 450 today. The average number of subscribers for each webinar is around 62, with a 90% effective presence. The webinars last little more than one hour and the Q&A session is usually very lively and quite informal.

The topics of the webinars, initially focused on the exploitation of Coherence of X-rays for inverse microscopy, have expanded to encompass other techniques exploiting coherence (e.g., XPCS, XCCA), analysis methods (e.g., phasing algorithms and the use of AI), instrumentation (e.g., beamlines worldwide providing access to these methods) and similar approaches in a different wavelength domain (e.g., high resolution microscopy with electrons and visible light).

All webinars are recorded and published in the educational platform of LINXS. This is an especially appreciated feature, people consistently ask for the recordings, and they are a source of high web-traffic. Two university professors (from Sweden and Denmark) have told Dina they use this database as their course material. On many occasions she gets attestations of appreciation for this series which has been also defined a “gift to the community interested in coherence”.

4. LINXS Strategic & Operational Achievements

This section reports on progress achieved towards the aims and objectives of LINXS for 2022 according to the LINXS Strategic and Operational Plan 2022 and follows the plan's headings for each objective.

➤ **Prepare for the move of LINXS to Science Village (SV).**

LINXS aims to be amongst the first settlers at Science Village (SV) so that it can engage with the local, national, and international developments on the site at an early stage. It has worked with various stakeholders (including the LINXS Board, the LU leadership and the leadership of the faculties of Science, Engineering and Medicine, several international organisations and facilities interested in SV, the Science Village Scandinavia office, the building companies constructing the first two buildings at SV, and, not least, researchers from Sweden and internationally, on the way the move could occur, the timing, the funding needed, and the possible tenancy arrangements. It also raised the interest of several organisations and initiated co-localisation discussions. Most importantly, LINXS has liaised with two building contractors and received very competitive offers for the location of LINXS at SV. The formal decision is expected in 2023.

➤ **Further develop LINXS as a vibrant, active, and attractive interdisciplinary community with a physical interaction hub near MAX IV and ESS.**

LINXS is now well established and known as a centre for advanced studies and education at local, national, and international levels. During 2022, LINXS has built on this, using

opportunities afforded by the appointment of the new Director and the transition from pandemic-state operations after March. In 2022, LINXS has:

- increased the number of activities and their type, by adding guest seminars/webinars, as well as collaborative/partner events (such as the BESS conference highlighted in Annex 6) and hosted events. All activities are listed in Annex 2. Furthermore, it has significantly increased the number of people involved, improved its operational routines, fully exploiting digital communications to optimise efficiency. As a result, the number of formally registered participants increased to 1717, from 1318 in 2021 and 526 in 2020. A conservative estimation is that over 2200 people have been involved in LINXS in some way during 2022, which is an increase from the previous year's 2000. The relative proportions of engagement are roughly the same across the various sectors, although we note a very significant increase in involvement from the LU Medical Faculty which has more than doubled. While the relative percentages are the same, the absolute number show a huge increase in engagement across the board. See "LINXS in numbers" (section 5) for more detail.
- set the visiting/guest researcher program more centrally in relation to the LINXS Themes, widened acceptance of Junior Guest Researchers (PhD students contributing to the Theme) – thus promoting the involvement of pioneering early-stage scientists, and tightened their involvement in LINXS activities.
- made LINXS a neutral attractive, comfortable, and stimulating environment to work in, physically and digitally, providing activities that promote interaction, discussion, and the development of ideas. The kick-off event after summer was held in an external location, stimulating a strong internal culture of collaboration. New employees in management and staff (including postdocs) have worked intensively and creatively. At the LINXS premises, offices were equipped to accommodate hot-desking of guests and collaborators, and hosting of events from other actors increased significantly. The first LINXS open day was held in December 2022.
- increased Newsletter output and professionalised communications and increased the promotion of activities related to science and research questions across the board. It increased production of articles by identifying, publicising, and disseminating the results, output, outcomes, and impact of LINXS Themes and activities (see under "LINXS communications as a pathway to impact").
- strengthened links to local, national, and international networks through collaborations, partnerships, and participation in projects when appropriate. LINXS has signed letters of support to project proposals and hosting of international events to be held in Lund between 2024-2027.
- further strengthened the digital capabilities related to remote and "hybrid" meetings. This has been a recipe for success during the pandemic and has heightened international reach and participation, as well as increasing the international impact of LINXS. Digital tools to curate, manage, and disseminate educational material and other online resources were acquired and human resources were assigned in the tasks to operate, capture and process digital events/recordings.
- Established itself as a "go to" place for information and events around X-ray and neutron-based and other infrastructure-linked research. This includes the curation of LINXS' own activities as well as joint events, partner activities, relevant events, and hosted events. The website was updated and a design for reorganisation was developed to include a calendar in the home page to facilitate quick finding of upcoming activities.

- Integrating further with MAX IV, ESS, other national and international LRIs and their outreach and training activities, e.g., user meetings, networks and jointly organise activities around new beamlines, methods, strategic objectives, or in-kind contributions. LINXS participated in the user meetings of MAX IV and ESS, the Swedish Physics Days, hosted several meetings and events (ESS and other including courses), and started coordinating/hosting the first Swedish in-kind project to ESS funded by the Swedish Research Council.
- **Extend LINXS' community including collaborations, partnerships, and memberships, emphasising the national and international scope.**

LINXS has progressed in consolidating and developing its community both nationally and internationally through strategic interactions, increased outreach activities in which the LINXS management took a more active role in representation and promotion, and a greater openness to joint events and hosted activities.

The pandemic has boosted wider participation and established LINXS as a respected international institute. This resulted in collaboration requests from national and international organisations to which LINXS was very positive when relevant to its mission statements.

Moreover, LINXS opened its first national and international Theme call in September allowing PIs from anywhere to apply for a LINXS Theme (see next point below).

Through the new IPDD Theme, and the visiting researcher programme (see relevant point below) the community of LINXS expanded further.

Finally, the RISE Large-Scale Research Infrastructures team continued to support LINXS as a member research group (see also "LINXS in numbers" below).

- **Promote and extend LINXS' scientific portfolio within and between the existing and new/developing Themes, exploiting the strong online capabilities that have emerged during the pandemic period.**
 - The Integrative Structural Biology Theme concluded its last activities during the year, and the Integrative Pharmacology and Drug Discovery (IPDD) Theme started on January 1st, 2022, with three working groups (see Annex 1). The "organic" practice of Themes developing from working groups and lively scientific interaction has continued, where several have been in the pipeline and applied in the new Theme Call 2022 in the end of the year.
 - LINXS developed "Legacy" webpages for the Themes that concluded and is open to support Theme sustainability after the incubation period as a LINXS Theme.
 - During 2022, LINXS transitioned to a post-pandemic state and increased the physical presence at its premises within safety guidelines. Communication effort was deployed to this end and some events were exclusively held in real life (IRL), whereas other expanded within a hybrid mode to maintain the new national/international public acquired. Cross-theme Town Hall meetings were developed as a purely on-line activity to put all Fellows in equal footing, regardless of their location in the world. This was highly appreciated for the increased cross-theme exchange of ideas and working practices.
 - LINXS used its experience in developing new theme research activities and beyond, by responding in a flexible way to external ideas and collaboration requests, as well as strategically invite guest speakers which served as inspiration and catalysed further interaction and new activities (see Annex 2).

- LINXS developed instructions, processes, templates, checklists and its online Handbook and Q&A, to facilitate the activities of working groups and help its Themes achieve the desired impact. An open position for a new Activities Coordinator was advertised at the end of the year. This has attracted a strong field of applicants and the outcome will be known in 2023.
 - Cross-theme activities have been encouraged as well as pioneering transdisciplinary efforts within and outside Themes. To this effect, LINXS has continued to develop its regular Science Day events, two of which were held in 2022 - all very well attended. Importantly, it initiated “Young Researchers Initiatives” in each of the LINXS focus areas, *i.e.*, hard matter, soft matter, and life sciences. These initiatives are designed to allow early-stage researchers to initiate and operate their own science events and is seen as part of a key LINXS goal to “nurture the PIs of the future”.
 - LINXS strove to keep all activities as nationally and internationally inclusive as possible, while maintaining resource efficiency. On-line participation was promoted, and unnecessary travel was avoided where it was strategically best and not detrimental to intended outcomes.
- **Establish new Themes of high scientific and societal relevance. Develop the working practices of active scientific Themes, and a strategy to open engagement of the national and international community.**
- During the year, LINXS worked on its strategic development and operations to establish a new Theme call model to widen participation nationally and internationally. This opens Themes to potentially being led from any national, or international, organisation according to a well-defined working model. The first national and international Theme call opened 2022-09-12 (F 2022/1895) attracting four new Theme applications by 2022-11-18, the deadline of the Stage 1 application process. The LINXS SAB evaluated these and the LINXS management subsequently invited the three lead applicants to submit a more comprehensive Stage 2 application in spring 2023.
 - LINXS aimed to have as many concurrent Themes running as possible within its available resources. Each Theme runs for a maximum of 3 years to enable a dynamic renewal of the community, activities, and outcomes. The new model for calls is expected to increase the available resources and thus the volume of Themes and activities. In addition, LINXS has submitted a *Centre of Excellence* application to the Swedish Research Council (VR). If successful, this will make LINXS a national platform, further increase the number of concurrent Themes, and make resources available to other Swedish universities (see also further down).
 - LINXS continued to develop call structures, topical directions (when appropriate) and specifics under the advice of the SAB. The new Theme call model was intensively discussed with the SAB and the Board.
- **Expand and improve the visitors program in line with the mission of LINXS.**

While the visiting researcher program was a success in 2019- early 2020, the pandemic stopped visits for most of 2022 and 2021. In 2021 LINXS worked towards restarting the program, and towards a strong list of potential visitors in coordination with the Themes and working groups, as well as pushing for an even stronger program in 2022. This of course was further compromised by the final pandemic in 2022. However, the first guest researchers were able to arrive in Lund in the summer. Three guest researchers came to LINXS in 2022. Jason Weaver worked with the New Materials Theme May - July, Jeremy Lakey worked with

the NLF Theme in June, and Elliot Gilbert, worked with the NLF Theme June – July. During these visits, Guest researchers took the opportunity to visit other Swedish universities. As the pandemic receded, LINXS worked intensively with the Themes to secure further growth in the number of visitors as early as possible in 2023.

In addition, from 2021 to 2022, LINXS hosted Dr Gudrun Lotze who has been working in collaboration with previous LINXS fellow Cedrick Dicko on a joint ESS and Uppsala University project aiming to improve the first future sample environment at the LoKI instrument at ESS. LoKI, which is a Small-Angle Neutron Scattering (SANS) instrument, will be one of the first instruments available to users at the ESS, which is set to open in 2026 (see Annex 6).

LINXS worked on strengthening the program and maximising the benefits for visiting scientists and the wider LINXS community. To this end, the guidelines for the visiting researcher program were refined to facilitate and encourage broader participation of guest researchers. Work was focused on:

- To make procedures for applying to be a guest researcher open and transparent.
- Publicising and highlighting the value of the visiting researcher programs and its impacts (including the use of the LINXS affiliation in publications) both to the external community and to the LINXS partners, making full use of the LINXS Newsletter.
- Investigation of funding opportunities to support the program, as this is clearly an attractive and visible activity.

➤ **Promote and facilitate education of both new and advanced users of X-ray and neutron methods with a view to the next generation of PIs.**

A key part of the LINXS mission is to educate both new and advanced users of ESS and MAX IV, as well as other Large-Scale Research Facilities and organisations. LINXS has coordinated numerous events to this end including webinar series and guest seminars, hosted courses and schools, as well as promoting external educational activities through its communication channels. LINXS has turned out to be an ideal location for doctoral schools and courses and LINXS encouraged external groups to run events at its premises, either as hosted or as partner events (see Annex 2). In 2022, LINXS:

- Developed education and training activities aimed at different levels and not just at the basic/introduction level.
- Continued to expand the educational material content on its website, including webinar videos, presentations from LINXS and LINXS-hosted events, links to external resources and developing material. By the end of 2022, the educational platform included more than 130 recorded talks, seminars, webinars and instructional videos. LINXS has solicited help from the LINXS postdoctoral fellows and other researchers to initiate restructuring work and develop instructional tools relevant to researchers at various levels of experience. The goal is to make the platform progressively more usable by developing the way the material is made available, so that users can easily match their knowledge level, and satisfy their ambition for knowledge and competence building.
- Worked with ESS and MAX IV towards workshops and education activities related to their beamlines and beamline development strategy. LINXS hosted numerous scientific and management groups from the facilities for their internal meetings; these will clearly profit from closer proximity when (hopefully) LINXS moves to the Science Village.

➤ **Actively encourage sustainability and gender balance in LINXS' operations.**

Sustainability. LINXS continues to encourage sustainable working practices. Vegetarian food is the default option at events, digital meetings are encouraged wherever appropriate. While LINXS is based around meeting and collaboration, travel needs are carefully evaluated. Remote conferencing is encouraged whenever possible and LINXS is fully equipped for such events. When possible, travel by train is prioritised. Furthermore, LINXS tries to organise guest seminars/webinars, and strategic meetings at the same time as other visits (e.g., visits to ESS or MAX IV) (see Annex 2).

Equality and diversity. LINXS considers gender balance and diversity in all its work. LINXS Themes were encouraged to arrange activities to attain a gender balance of at least 60%-40%. The same general aim exists for diversity in panels and amongst invited speakers. There was a slight worsening of the gender balance during 2022 to a 34%/66% female/male ratio, from an improved 36%/64% in 2021 which was up from 24%/76% in 2020 (see LINXS in number below). LINXS will continue to press this priority for gender balance in 2023 and beyond.

- **Develop the branding of LINXS to reflect the breadth of its national and international engagement and to disseminate and to publicise its impact and added scientific value.**

LINXS progressed very well in this area during the year and has successfully identified itself on the scientific scene both nationally and internationally. This is increasingly evident from the composition of the guest and Theme activities, the feedback received during meetings with national and international organisations, such as universities in Sweden, facilities in Sweden and abroad, and Swedish authorities (e.g., Swedish Research Council), at various strategic levels.

LINXS is not inward-looking and is committed to the full exploitation of two major facilities – MAX IV (national) and ESS (international) on behalf of the whole country. It has made this clear to the research communities throughout the country:

- by developing and submitting a Centre of Excellence (CoE) application to VR with letters of support from top leadership of both MAX IV and ESS, as well as from a large number of Swedish universities. A LINXS CoE will be able to support Swedish universities in developing thematic areas, with their relevant research communities benefiting Swedish scientific excellence and making the most out of the facilities at a national level. Results on whether the LINXS CoE will be funded in 2024-2029 will be known in the middle of 2023.
- through direct engagement with other Swedish universities in a manner that facilitated access and collaboration with MAX IV, ESS.
- through the modification of the eligibility rules for the creation of new Themes where LINXS opened the first national and international call for new Themes in the end of 2022.
- by evolving the branding of LINXS to remove any perception of local bias. The branding of the institute has been very effective, and the prior perception across Sweden and even internationally that LINXS served Lund exclusively was eliminated removing LINXS as an acronym and changing it to “LINXS Institute of advanced Neutron and X-ray Science”. This has been met with wide general enthusiasm!

Furthermore, LINXS increased its communication engagement as part of a continuous, active, and strategic effort (see below under “LINXS communications as a pathway to impact”).

➤ **Engage board and management group members towards more effective development and operation of LINXS.**

During 2022, Olof “Charlie” Karis, the national representative to the LINXS Board, needed to leave his engagement following his new role as Director of MAX IV. Given the importance of an active national representative in anchoring LINXS with Swedish universities, Anders Karlhede from Stockholm University was appointed as the national representative in June 2022. This appointment followed the same transparent process through nominations from the Swedish Universities’ Reference Group for Research Infrastructure (URFI). The involvement of URFI strengthens the national perspective of LINXS and the value it brings nationally.

Furthermore, LINXS has engaged its Board more in its decision-making; Board meetings have involved more detailed discussion rather than being a forum for reporting by the management. The LINXS Director/Management continued to liaise with the board and its Chair for the working practices and activities of LINXS, as well as on the strategic initiatives and actions such as the move to new LINXS premises at Science Village. This level of engagement with the Board will be essential in the future as LINXS develops strategic collaboration with national universities/institutes.

The LINXS Management Group which started in 2022 worked together with the Director on defining clear roles and responsibilities for the management. Work is ongoing. Moreover, work needs to progress in developing the “ambassador” role of the Management members nationally and internationally through concrete actions.

➤ **Engage the Scientific Advisory Board and work on the renewal of the membership towards ensuring the scientific excellence of LINXS.**

Twice in 2022, LINXS has had formal reviews by its Scientific Advisory Board (SAB). The SAB convened in May and December where it also evaluated the Theme applications received in the first LINXS national and international Theme call.

The SAB gave valuable feedback on the process of the Themes and their activities. LINXS works closely with its SAB and benefits greatly from its experience and wide range of competence.

Two new SAB members were appointed during the year to substitute departing members and SAB member Prof. Christiane Alba-Simionesco was appointed as the interim chair since the existing chairman needed to take leave for personal reasons.

➤ **Secure medium and long-term funding, as well working towards new funding opportunities/applications (e.g., foundation funding and EU).**

Funding has been secured for 2021-2025 from the LU NMT faculties, and centrally from the vice-chancellor) until 2024.

The possibility of establishing LINXS as a “USV” is a standing discussion item at LINXS Board meetings. There are various arguments that weigh into this discussion that relate to the local/national roles and management of LINXS. However, for the moment LINXS is well hosted by the Chemistry Department. A thorough cost-benefit analysis will be needed to establish the strategic and political consequences of such a change. This was not prioritised during 2022.

Funding from sources other than LU is essential for the growth and development of the institute and to bring about impact that will propel the next generation researchers as the new PIs of the large infrastructures. Therefore, external funding opportunities were investigated to fund both the new national and international model of LINXS, as well as to support PhD students and postdoctoral allowing them to engage with LINXS-related activities.

As mentioned, LINXS applied for funding to VR with a CoE application using the basic LU funding as co-funding leverage. In parallel, LINXS supported applications for courses, schools, and large conferences as a partner, offering its premises and administrative support. One such partnership is "NNSP PhD School in Neutron Scattering" which got awarded in December up to funding 4 000 000 NOK by NordForsk.

Progressing in establishing itself within EU funded initiatives (either as lead or partner), LINXS also started developing a proposal under the EU MSCA COFUND programme to coordinate the recruitment of many postdoctoral researchers with a deadline in spring 2023.

LINXS still needs to work with NMT and LU to develop strategies towards funding from foundations. There exists the possibility to approach Region Skåne, but a relevant action did not mature in 2022. Finally, LINXS should also work to establish itself within EU funded initiatives (either as lead or partner).

Funding acquired from the LMK foundation allowed the employment of a LINXS LMK Postdoc (see relevant report above). LINXS has also been directly involved in the GISANS initiative, with a postdoc being placed at LINXS to carry out the work.

Regarding to the sustainability of Themes, project-based funding has been a major NLF achievement, as detailed in the Theme report above.

4.1. Communications as a pathway to impact

LINXS continued to use communications and outreach strategically towards realising the overall mission. Focus lays on identifying and promoting the benefits, outputs and added value of LINXS through various channels.

As the activities of LINXS increases and extends to more areas and communities, the significance of capturing and giving value to the various outputs is growing. This is an ongoing effort, and a concrete communication plan is followed every year as a strategic pathway to achieve long lasting scientific and societal impact short, medium, and long term. Strategic outreach activities (see Annex 2) served to promote the LINXS science and strengthen the LINXS identity in both local, national, and international contexts.

News highlights

Important highlights during the year include the announcement of the new Theme, Integrative Pharmacology and Drug Discovery (IPDD), and connected Theme activities such as different workshops by various working groups. Some of these activities were also highlighted in Lund University faculty channels.

LINXS also focused on capturing the last ISB conference, the Time Resolved Structural Biology workshop - final event within the ISB Theme, as well as the thematic activities within

the New Materials and Northern Lights on Food Themes, with a view to highlight how Themes are pushing scientific discussions forward.

LINXS also interviewed guest researchers, and international researchers visiting LINXS to hold guest seminars. These activities are part of the efforts to highlight important developments, people and happenings connected to the broader X-ray and neutron communities, and large-scale infrastructures world-wide. 2022 was the first year where key guest speakers were invited to give hybrid seminars at LINXS. The aim was not only knowledge dissemination, but also networking and anchoring the institute with key international organisations to promote future collaboration opportunities.

Newsletters and news articles

Publication of the LINXS newsletter continued, and subscriptions increased to 2.650, up from 2.179 the year before. Six newsletters were issued in 2022. The main aim is to showcase LINXS work, activities, and Themes to internal and external target groups – with a view to stimulate interest and excitement, both in LINXS and in X-ray and neutron science. It also aims to attract interest for scientific collaborations and to entice other organisations towards joining the LINXS initiative through partnerships. Moreover, the newsletter serves to strengthen the LINXS identity in local, national, and international contexts.

LINXS changed newsletter provider during the year, so the following statistics are based on five newsletters: on average 834 people opened each newsletter, ranging from 793 to 903 persons, an average of 37,4 % opening rate. This rate is very good, considering the increased subscriptions, and shows that the work of LINXS and its thematic activities are perceived as relevant to the LINXS community and beyond.

LINXS communicated activity results also through a series of popular science articles about LINXS Themes and working group work, capturing output, value, and impact potential. These articles were included in the newsletters and the website. In total, 42 news articles were produced (including announcements, Theme calls, LINXS webinar series, LINXS newsletter and popular science articles). The aim of such articles is to contribute towards increasing awareness about the work of LINXS, showcase ongoing X-ray and neutron science and maintain the interest of researchers already invested in LINXS.

Key points include highlighting the science at LINXS and the community building, plus demonstrating the value-added, scientific relevance and quality.

Event marketing

As the activities of LINXS continued to expand, LINXS focused on increasing its marketing activities during the year. Using a targeted newsletter tool, which is also used for LINXS newsletter, targeted information emails for the majority of LINXS events were sent out starting in autumn. These targeted emails increased participation numbers, and awareness of LINXS events, and is a complement to the newsletters and marketing on social media. With their professional layout, the marketing emails also serve to further brand LINXS and its Theme activities to key target groups.

Website

The LINXS website is the main tool for communication about its work and remit. It continued to be updated and expanded during the year, with a focus on supporting current and potential researchers at LINXS.

The LINXS website had 34.719 visits in 2022, an increase of 24 % compared to 2021. 23.868 out of these were unique visitors, representing a 24 % increase. It also had 64.327 page views, an increase of 13 %. Most popular content in descending order were the “Home” page, the LINXS “events” page, the Northern Lights on Food Theme page, and the “Management” page. There is also a noticeable increase of the views of the educational materials platform.

Social media

The LINXS YouTube channel was updated with a new introductory film about LINXS to reflect the change of the LINXS name and logo. During the year recording of webinars such as LINXS guest seminars, and presentation from Theme events continued to be uploaded.

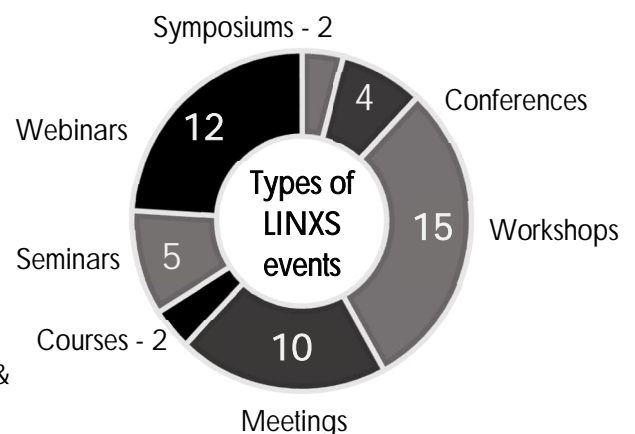
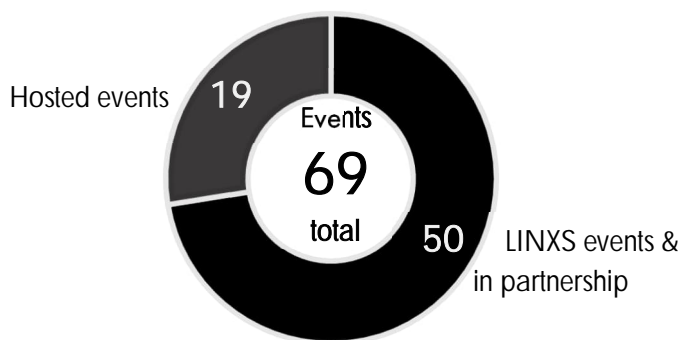
The LINXS Twitter account @LINXS_Sweden expanded its follower base to 420 persons and organisations and is actively following 353 key actors and persons in the field. Retweets have gradually increased.

The LINXS LinkedIn page was developed to further promote all articles, newsletters, and events, gaining an increased number of followers amounting to 1.164 persons (an increase of 30 % as compared to 2021). The social media platform continues to serve as an important communication tool, and the fact that followers are growing in number is a testament to the usefulness and perceived value of this communication channel. In addition, followers are becoming more active in reposting, sharing, and commenting, contributing in this way to the increased spread of the LINXS information and activities.

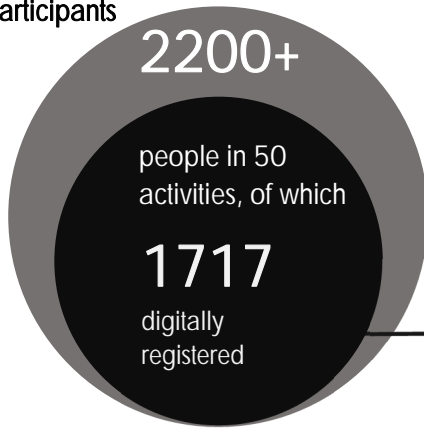
Some activities outlined in the LINXS communication plan 2022 were not completed. They include training on impact for the LINXS community, and the proposed interviews of key people in LINXS Themes and working groups. The aim of the interviews is to assess how LINXS communication efforts are perceived. These activities will be undertaken in 2023 or later, based on managerial prioritisation as LINXS expands and further develops.

5. LINXS in numbers 2022

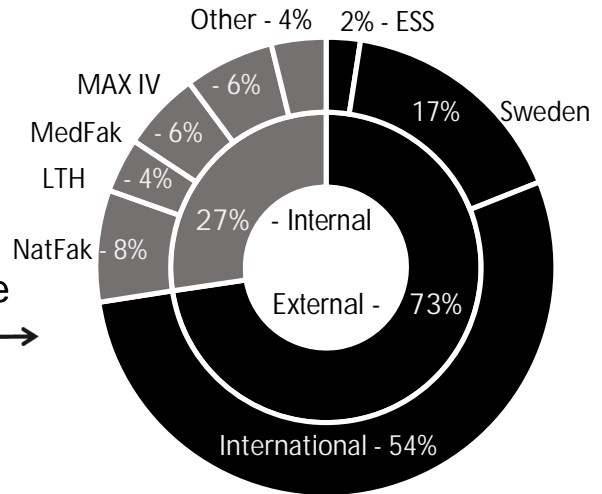
LINXS Activities and participation



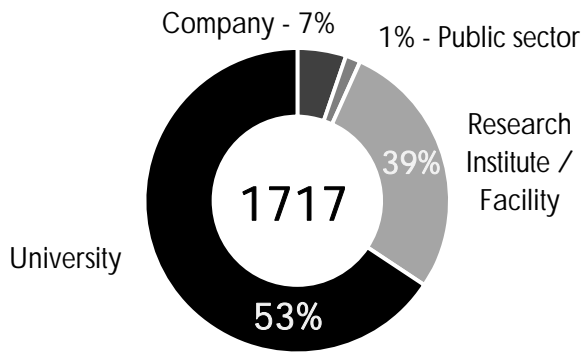
Participants



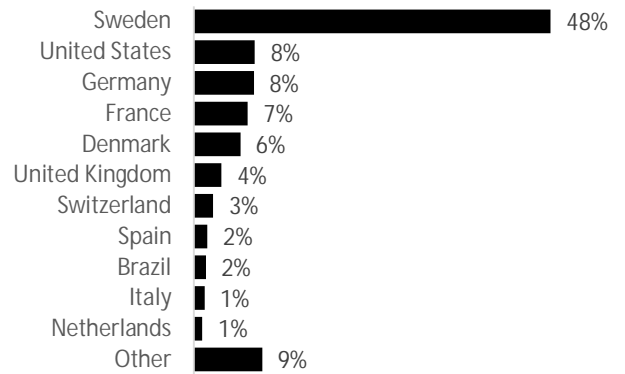
of these



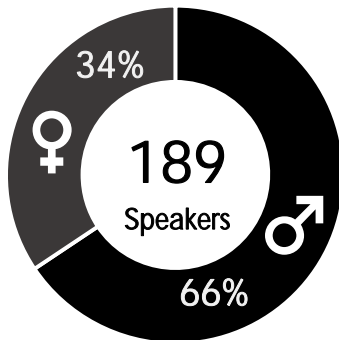
Organisational types



Country of origin

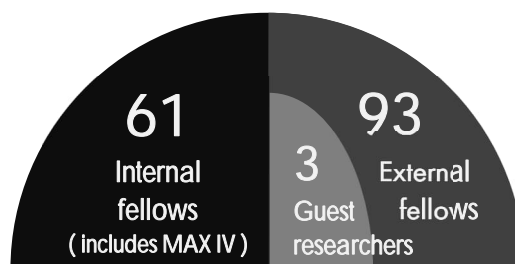


Keynote speakers' gender balance



LINXS Community – fellows in 2022

154 LINXS fellows in 2022



LINXS Community - affiliations of LINXS fellows

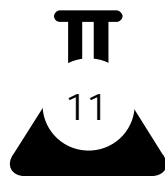
58 organisations are involved in the LINXS core groups, working groups, and visiting researcher programme.

22 in Sweden (including Lund University)

36 international AUS:2, CH:1, DE:9, DK:6, ES:4, FI:2, FR:3, IT:1, LU:1, NO:1, UK:4, US: 2



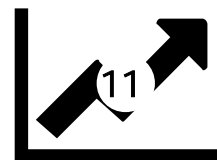
Universities



Research Institutes



Large Scale
Research Infrastructures



Companies

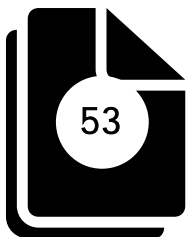


2 Core Partners (ESS and MAX IV in addition to Lund University)

1 Member (Research Group)

10 Collaborations

Outcomes



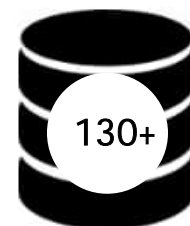
Publications with
LINXS affiliation



Project applications



Projects funded



Educational Records

21 additional publications were reported by the Themes but had no formal affiliation.

Communications



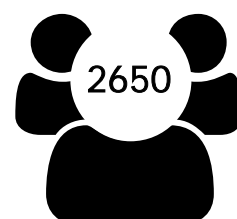
Outreach activities



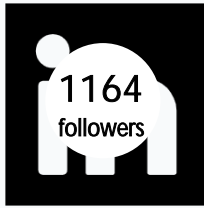
Website news



Newsletters



Subscribers



LinkedIn



Twitter

6. Annual Financial Report 2022

Income	SEK
Conference fees	380,927
External funding	1,549,717
Partners contribution	8,500,000
Membership fees	50,000
Total Income 2022	10,480,644
Expenditures	SEK
Activities	-1,417,755
Equipment	-76,402
Materials & consumables	-299,595
Premises	-1,235,658
Salaries	-5,062,700
Overhead	-1,645,116
Total Expenditures	-9,737,226
Annual Result 2022	743,418

Partner contributions during 2022 was funding from the Lund University Central administration and the faculties of Science, Engineering and Medicine at Lund University. The faculty of Medicine also contributed in-kind with 20% of the salary of the LINXS co-director and 20% of the salary of the IPDD Theme leader. The final surplus is moved to the 2023 budget together with the accumulated agency capital from the previous years.

Detailed financial reporting is included in Annex 5.

Annex 1 – LINXS Themes and Working Groups in 2022

INTEGRATIVE STRUCTURAL BIOLOGY (ISB) – CONCLUDED

Theme and Core Group Leader: Karin Lindkvist, Lund University, Sweden

WG 1 - Biocompute and Artificial Intelligence & Machine Learning (concluded)

WG 2 - Time-Resolved Structural Biology - New possibilities in a time of new facilities

Leader – Thomas Ursby, MAX IV, Lund University, Sweden

WG 3 - Amyloid: An integrative approach

Leader – Oxana Klementieva, Lund University, Sweden

WG 4 - Membrane Proteins - Structural resolution and homology modelling

Leader – Urban Johanson, Lund University, Sweden

WG 5 - Lund Integrative Structural Biology Centre Initiative (LISBC)

Leader – Karin Lindkvist, Lund University, Sweden

NEW MATERIALS

Theme and Core Group Leader: Elizabeth Blackburn, Lund University, Sweden

WG 1 - Functional Magnetic Materials

Leader – Elizabeth Blackburn, Lund University, Sweden

WG 2 - Charge Transfer Materials (fused with WG 3)

WG 3 - Light Harvesting Processes

Leader – Jens Uhlig, Lund University, Sweden

WG 4 - Catalysis

Leader – Sara Blomberg, Lund University, Sweden

WG 5 - Nanostructures and Interfaces

Leader – Maria Messing, Lund University, Sweden

NORTHERN LIGHTS ON FOOD (NLF)

Theme and Core Group Leader: Selma Maric, Lund University, Sweden and Tommy Nylander, Lund University, Sweden (from August 2022)

WG 1 - Structure of food raw materials

Leader – Francisco Vilaplana, KTH, Sweden

WG 2 - Food colloids and structured interfaces

Leaders – Ben Boyd and Jacob Kirkengaard, Copenhagen University, Denmark

WG 3 - Structure of food during processing

Leaders – Stephen Hall, Lund University and Niklas Lorén, RISE, Sweden

WG 4 - Food interactions on surfaces

Leader – Jenny Schelin, Lund University, Sweden

WG 5 - Food structure and health

Leader – Peter Spéjel, Lund University, Sweden

INTEGRATIVE PHARMACOLOGY AND DRUG DISCOVERY (IPDD)

Theme and Core Group Leader: Karin Lindkvist, Lund University, Sweden

WG 1 - Structure-based drug design

Leader – Raminta Venskutonytė, Lund University, Sweden

WG 2 - Macromolecular Drugs –Antibodies

Leader – Anna Stradner, Lund University, Sweden

WG 3 - Biomedical Imaging

Leader – Lars E. Olsson, Lund University, Sweden

Annex 2 – List of LINXS activities 2022

LINXS Guest Researcher Programme:

1. Jason Weaver, LINXS Guest researcher May - July 2022 (New Materials)
2. Jeremy Lakey, LINXS Guest researcher June 2022 (NLF)
3. Elliot Gilbert, LINXS Guest researcher June - July 2022 (NLF)

LINXS events and events organised in partnership:

1. Northern Lights on Food LU Profile Area Workshop, Jan 12-13, 2022 (NLF)
2. LINXS partner event – Kick-off SAGA – Preparing for a GISANS instrument at ESS – A Swedish Initiative, Jan 14, 2022 (SAGA GISANS)
3. LINXS event – Food WG5 Webinar on the study of lipid structures in membranes and food formulations, Feb 8, 2022 (NLF)
4. 2nd workshop Metals and manufacturing @ next generation sources - Partner event, Mar 10, 2022
5. LINXS event - WEBINAR: CoWork series – Structural evolution of nanoparticles under realistic conditions observed with Bragg coherent X-ray imaging with Marie-Ingrid Richard, Mar 10, 2022
6. Food WG4 meeting, Mar 18, 2022 (NLF)
7. LINXS event - WEBINAR: CoWork series – Single-particle diffraction imaging at the European XFEL with Filipe Maia, Mar 24, 2022
8. LINXS event - WEBINAR: CoWork series – Coherent X-ray diffraction imaging at Nanoscale with Ivan A. Vartanyants, Apr 7, 2022
9. LINXS partner event – 18th Food colloids digital conference: Structure, Dynamics and Function, Apr 10-13, 2022 (NLF)
10. ISB Core group, pre-symposium meeting (ISB)
11. LINXS event – Northern Lights on Food 3D hackathon, Apr 27-28, 2022 (NLF)
12. LINXS event – LINXS Science Day – rebooting from the pandemic, Apr 29, 2022
13. LINXS event – IPDD Kick-off meeting, May 2, 2022 (IPDD)
14. LINXS event – 3rd Integrative Structural Biology Symposium, May 4-6, 2022 (ISB)
15. LINXS event – Imaging Workshop: Imaging possibilities for Breakthrough in medical research, May 11, 2022
16. LINXS event – Food WG 4 Workshop, May 11, 2022 (NLF)
17. LINXS event - Workshop: Northern Lights on Food III, Jun 1-3, 2022 (NLF)
18. US Delegation visit to Lund, Jun 5, 2022 (NLF)
19. LINXS event - WEBINAR: CoWork series – Magnetic chirality in multilayers probed by Soft X-ray (coherent) scattering, with Nicolas Jaouen, Jun 9, 2022
20. NLF WG4 meeting with Guest professor Jeremy Lakey, Jun 9, 2022
21. LINXS event - Workshop: Magnetic SANS – Data Analysis and Software Prospects, June 13-14, 2022 (New Materials)
22. LINXS partner event – Lipid Bilayers at ESS – BESS in Lund, Jun 13-15, 2022
23. LINXS event – SasView CodeCamp (ESS), June 14-16, 2022 (New Materials)
24. Swedish Physics Days in Lund, Jun 15-17, 2022 (New Materials)
25. LINXS Guest Seminar – D.D Sarma, Indian Institute of Science (IISc), Bangalore, Jun 16, 2022

26. LINXS event - WEBINAR: CoWork series – Atomic Resolution Imaging by Electron Ptychography with David A. Muller, Jun 16, 2022
27. LINXS event – Workshop – Catalysis Workshop, Jun 30, 2022 (New Materials)
28. LINXS event – Masterclass: 3rd Northern Lights on Food Masterclass, Aug 29-Sep 2, 2022 (NLF)
29. LINXS event - WEBINAR: CoWork series – Recent developments on Bragg ptychography with Peng Li, Sep 15, 2022
30. Chemistry of Life Joint Symposium University of Leicester and LU, Sep 23, 2022
31. LINXS event – Antibodies MoB meeting mAb Midterm Meeting 2022, Sep 27-28, 2022 (IPDD)
32. LINXS event – LINXS Science Day – Imaging and Dynamics, Sep 28-29, 2022
33. LINXS event - WEBINAR: CoWork series – Complexity and Local Heterogeneity by Coherent X-ray Diffraction Imaging with Hyunjung Kim, Sep 29, 2022
34. LINXS event – Food Colloids and Structured Interfaces Industry Workshop NLF WG 2, Oct 4, 2022 (NLF)
35. LINXS partner event – Saga Gisans update meeting in connection to MAX IV & ESS user meetings, Oct 4, 2022 (SAGA GISANS)
36. LINXS partner event – HELIOS research school, Oct 10-14, 2022
37. LINXS event - WEBINAR: CoWork series: A new Bragg Coherent Diffractive imaging beamline at NSLS.II, with Garth Williams, Oct 13, 2022
38. LINXS Northern Lights on Food Theme Meeting at ESS and LINXS, Vinnova-project: Strengthened research and innovation in the food sector made possible by neutron and synchrotron techniques, 2021-0409-NLF, Oct 17-18, 2022 (NLF)
39. LINXS event – Workshop on Biomedical Imaging for drug discovery/development – Opportunities for MAX IV, Oct 19, 2022 (IPDD)
40. LINXS Partner event – Joint LINXS/Physical Chemistry/KILU/Food Technology, engineering, and Nutrition seminar: Leoni Van't Hag, Oct 19, 2022 (NLF)
41. LINXS Event – TRSB Final workshop – 2nd Time-Resolved Structural Biology Workshop, Oct 26-28, 2022 (ISB)
42. LINXS event - WEBINAR: Antibodies in Solution: a LINXS-NIST webinar series – Therapeutical monoclonal antibodies- significance for patients and evolution into the future with Karoline Bechtold-Peters, Oct 2, 2022 (IPDD)
43. NLF WG5 Webinar - Dr Marta Martinez-Sanz, Prof. Judith Peters, Nov 7, 2022 (NLF)
44. NLF Guest Seminar - Izabela Milogrodzka, Nov 8, 2022 (NLF)
45. LINXS event – IPDD – Structure based drug design meeting, Nov 14-15, 2022 (IPDD)
46. LINXS event – LINXS virtual Town Hall meeting, Nov 29, 2022
47. LINXS Guest Seminar - Paul Langan Director General of the Institute Laue Langevin, Nov 30, 2022
48. LINXS Guest Seminar - Robert McGreevy, Dec 2, 2022
49. LINXS event - WEBINAR: Antibodies in Solution: a LINXS-NIST webinar series - John Schiel, Dec 7, 2022 (IPDD)
50. LINXS Christmas Open House, Dec 15, 2022

LINXS Hosted activities:

1. Research Group meeting, Theoretical Chemistry, Feb 16, 2022
2. Magnet reference group, Mar 23, 2022 (NLF)
3. RÅC governing committee meeting, May 4, 2022

4. Research Group meeting, Theoretical Chemistry, May 18, 2022
5. Summer School Structural biology, LINXS - MAX IV "MicroMAX Masterclass - Summer School. HALOS-EUGLOH Summer School 2022, Jun 6-7, 2022
6. N-fak Faculty Board meeting, Jun 6, 2022
7. BiSS@LU Contributions to RIs, Jun 23, 2022
8. ESS instrument scientists' "Science Afternoon at LINXS", Jun 29, 2022
9. N-fak Faculty Board meeting, Aug 18, 2022
10. ESS instrument scientists' "Science Afternoon at LINXS", Aug 30, 2022
11. 5th Nordic/Baltic school of neutron scattering NNSP SwedNess, Sep 3-12, 2022
12. SuperADAM board meeting – NLF, Oct 10, 2022
13. SESAM project meeting, Oct 25, 2022
14. SwedNess Sall-Angle Neutron Scattering (SANS) Research school on neutrons, Nov 7-11, 2022
15. Nanolund Career development workshop, Nov 17, 2022
16. LU Collaboration department meeting, Nov 23, 2022
17. ESS scientist away day, Nov 25, 2022
18. COMPUTE Jupyter Course, Dec 6-9, 2022
19. LU Collaboration department meeting, Dec 14, 2022

LINXS Outreach activities:

1. SXNS16 Conf - LINXS (digital), Jan10-14, 2022
2. MAX IV - UPPSALA meeting, Apr 7, 2022
3. DTI visit, Apr 21, 2022
4. ISB meeting with Leicester University, May 3, 2022 (ISB)
5. Swedish Neutron Week 2022, May 16-19, 2022
6. HALOS Final Conference, Jun 8, 2022
7. Chemical Society SCS 2022, Jun 20
8. Northern Lights on Food at Innovation week, Jun 23, 2022
9. Connecting LINXS and ISBUC meeting, Aug 8, 2022
10. Director visit to Uppsala, Sep 21, 2022
11. 34th MAX IV User meeting "Collaboration in Focus", Oct 3-5, 2022, LINXS stand
12. ESS and ILL European Users meeting, Oct 5-7, 2022, LINXS stand
13. Visit to LINXS of Eric Cassan, deputy vice-president from University of Paris-Saclay (EUGLOH), Nov 16, 2022
14. Learning meeting about the societal benefit of the research facilities ESS and MAX IV, Nov 22, 2022
15. ESS/MAX IV Summit 2022
16. SVS open house, Dec 14, 2022

Annex 3 – List of publications with LINXS affiliation 2022

LINXS affiliated publications that have been communicated to LINXS. LINXS fellows are encouraged but not obliged to use the LINXS affiliation, or to acknowledge LINXS when credit is due.

1. **Correlative optical photothermal infrared and X-ray fluorescence for chemical imaging of trace elements and relevant molecular structures directly in neurons.** Nadja Gustavsson, Agnes Paulus, Isak Martinsson, Anders Engdahl, Kadda Medjoubi, Konstantin Klementiev, Andrea Somogyi, Tomas Deierborg, Ferenc Borondics, Gunnar K Gouras, Oxana Klementieva. *Light Sci Appl.* 2021 Jul 22;10(1):151. doi: 10.1038/s41377-021-00590-x.
2. **Kitchen-Based Light Tomography - a DIY toolkit for advancing tomography - by and for the tomography community.** Emanuel Larssona, Doğa Gürsoy, Stephen A. Hall, (2022) *Tomography of Materials and Structures*
3. **Report on the Workshop on “Magnetic Small Angle Neutron Scattering - Data Analysis and Software Prospects.** Annika Stellhorn, Wojciech Potrzebowski & Paul D. Butler, (2022) *Neutron News*, 33:4, 9-10.
4. **Statistical thermodynamics in reversible clustering of gold nanoparticles. A first step towards nanocluster heat engines.** Stefano A. Mezzasalma, Joscha Kruse, Amaia Iturraspe Ibarra, Arantxa Arbe, Marek Grzelczak, 2022: *Journal of Colloid and Interface Science*, Volume 628, Part A, 15 December 2022, Pages 205-214
5. **Rubber elasticity of polymer networks in explicitly non-Gaussian states. Statistical mechanics and LF-NMR inquiry in hydrogel systems.** Stefano A. Mezzasalma, Michela Abrami, Gabriele Grassi, Mario Grassi, 2022: *International Journal of Engineering Science*, Volume 176, 1 June 2022, 103676.
6. **Probing cage relaxation in concentrated protein solutions by XPCS.** Chushkin Y., Gulotta A., Roosen-Runge F., Pal A., Stradner A., Schurtenberger P. arXiv:2203.12695 [cond-mat.soft] 2022.
7. **Probing Cage Relaxation in Concentrated Protein Solutions by X-Ray Photon Correlation Spectroscopy.** Yuriy Chushkin, Alessandro Gulotta, Felix Roosen-Runge, Antara Pal, Anna Stradner, and Peter Schurtenberger. *Phys. Rev. Lett.* 129, 238001 – Published 29 November 2022.
8. **A modified Jarzynski free-energy estimator to eliminate non-conservative forces and its application in nanoparticle-membrane interactions.** Hosseini, A. N., Lund, M. & Ejtehadi, M. R., 2022 feb. 14, I: *Physical Chemistry Chemical Physics*. 24, 6, s. 3647-3654 8 s.
9. **Anion-cation contrast of small molecule solvation in salt solutions.** Hervø-Hansen, S., Heyda, J., Lund, M. & Matubayasi, N., 2022 feb. 7, I: *Physical Chemistry Chemical Physics*. 24, 5, s. 3238-3249 12 s.
10. **Assessing the structural and dynamical properties of concentrated solutions of the disordered proteins Histatin 5 and its tandem repeat.** Fagerberg, E., 2022, Lund University. 258 s.

11. **C-amidation of substituted β 3oligoamides yields novel supramolecular assembly motif.** Buchanan, C., Puskar, L., Garvey, C. J. & Mechler, A., 2022 jan. 8, I: Nanotechnology. 33, 2, 025601.
12. **Characterisation of Grains and Flour Fractions from Field Grown Transgenic Oil-Accumulating Wheat Expressing Oat WRI1.** Snell, P., Wilkinson, M., Taylor, G. J., Hall, S., Sharma, S., Sirijovski, N., Hansson, M., Shewry, P. R., Hofvander, P. & Grimberg, Å., 2022 apr., I: Plants. 11, 7, 889.
13. **Clustering and cross-linking of the wheat storage protein α -gliadin: A combined experimental and theoretical approach.** Markgren, J., Rasheed, F., Hedenqvist, M. S., Skepö, M. & Johansson, E., 2022, I: International Journal of Biological Macromolecules. 211, s. 592-615 24 s.
14. **Correlative imaging to resolve molecular structures in individual cells: Substrate validation study for super-resolution infrared microspectroscopy.** Paulus, A., Yogarasa, S., Kansiz, M., Martinsson, I., Gouras, G. K., Deierborg, T., Engdahl, A., Borondics, F. & Klementieva, O., 2022, I: Nanomedicine: Nanotechnology, Biology and Medicine. 43, s. 102563 102563.
15. **Counterintuitive Electrostatics upon Metal Ion Coordination to a Receptor with Two Homotopic Binding Sites.** Aspelin, V., Lidskog, A., Solano Arribas, C., Hervø-Hansen, S., Stenqvist, B., Chudoba, R., Wärnmark, K. & Lund, M., 2022 feb. 10, I: Journal of the American Chemical Society. 144, 7, s. 2921-2932 12 s.
16. **Early-life stress elicits peripheral and brain immune activation differently in wild type and 5xFAD mice in a sex-specific manner.** Bachiller, S., Hidalgo, I., Garcia, M. G., Boza-Serrano, A., Paulus, A., Denis, Q., Haikal, C., Manouchehrian, O., Klementieva, O., Li, J. Y., Pronk, C. J., Gouras, G. K. & Deierborg, T., 2022 juni 15, I: Journal of Neuroinflammation. 19, 151.
17. **Effect of encapsulated protein on the dynamics of lipid sponge phase: a neutron spin echo and molecular dynamics simulation study.** Gilbert, J., Ermilova, I., Nagao, M., Swenson, J. & Nylander, T., 2022, (E-pub ahead of print) I: Nanoscale.
18. **Electronic polarization effects on membrane translocation of anti-cancer drugs.** Najla Hosseini, A., Lund, M. & Ejtehadi, M. R., 2022 apr. 18, I: Physical Chemistry Chemical Physics. 24, 20, s. 12281-12292 12 s.
19. **Fibre directions at a branch-stem junction in Norway spruce: a microscale investigation using X-ray computed tomography.** Hu, M., Olsson, A., Hall, S. & Seifert, T., 2022, I: Wood Science and Technology. 56, 1, s. 147-169
20. **From dilute to concentrated solutions of intrinsically disordered proteins: Sample preparation and data collection.** Lenton, S., Tully, M. D. & Skepö, M., 2022 okt., (E-pub ahead of print) Methods in Enzymology. Academic Press, 22 s.(Methods in Enzymology).
21. **Impact of Compression on the Electrochemical Performance of the Sulfur/Carbon Composite Electrode in Lithium-Sulfur Batteries.** Chien, Y. C., Li, H., Lampkin, J., Hall, S., Garcia-Araez, N., Brant, W. R., Brandell, D. & Lacey, M. J., 2022, I: Batteries and Supercaps. 5, 7

22. **Innovative Green Way to Design Biobased Electrospun Fibers from Wheat Gluten and These Fibers' Potential as Absorbents of Biofluids.** Muneer, F., Hedenqvist, M. S., Hall, S. & Kuktaite, R., 2022, I: ACS Environmental Au. 2, 3, s. 232-241
23. **Innovatively processed quinoa (*Chenopodium quinoa* Willd.) food: chemistry, structure and end-use characteristics.** Kuktaite, R., Repo-Carrasco-Valencia, R., de Mendoza, C. C. H., Plivelic, T. S., Hall, S. & Johansson, E., 2022, I: Journal of the Science of Food and Agriculture. 102, 12, s. 5065-5076
24. **In situ microstructural evolution of spruce wood during soda pulping using synchrotron X-ray tomography.** Wagih, A., Hasani, M., Hall, S. A., Novak, V. & Theliander, H., 2022, I: Holzforschung. 76, 7, s. 611-621
25. **Interaction of nanoparticles with lipid films: The role of symmetry and shape anisotropy.** Caselli, L., Ridolfi, A., Mangiapia, G., Maltoni, P., Moulin, J. F., Berti, D., Steinke, N. J., Gustafsson, E., Nylander, T. & Montis, C., 2022 feb. 7, I: Physical Chemistry Chemical Physics. 24, 5, s. 2762-2776 15 s.
26. **Interactions Between Imbibition and Pressure-Driven Flow in a Microporous Deformed Limestone.** Lewis, H., Couples, G., Tengattini, A., Buckman, J., Tudisco, E., Etxegarai, M., Viggiani, G. & Hall, S. A., 2022, (E-pub ahead of print) I: Transport in Porous Media.
27. **Localised strain in fissured clays: The combined effect of fissure orientation and confining pressure.** Tudisco, E., Vitone, C., Mondello, C., Viggiani, G., Athanasopoulos, S., Hall, S. A. & Cotecchia, F., 2022, I: Acta Geotechnica. 17, 5, s. 1585-1603
28. **Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction.** Drago, V. N., Devos, J. M., Blakeley, M. P., Forsyth, V. T., Kovalevsky, A. Y., Schall, C. A. & Mueser, T. C., 2022, I: npj Microgravity. 8, 1, 13.
29. **Microscale deformation mechanisms in paperboard during continuous tensile loading and 4D synchrotron X-ray tomography.** Johansson, S., Engqvist, J., Tryding, J. & Hall, S. A., 2022, I: Strain. 58, 5
30. **Molecular dynamics simulations of the adsorption of an intrinsically disordered protein: Force field and water model evaluation in comparison with experiments.** Koder Hamid, M., Månsson, L. K., Meklesh, V., Persson, P. & Skepö, M., 2022 okt., I: Frontiers in Molecular Biosciences. 9, 14 s., 958175.
31. **Nanoscale structural and mechanical characterization of thin bicontinuous cubic phase lipid films.** Ridolfi, A., Humphreys, B., Caselli, L., Montis, C., Nylander, T., Berti, D., Brucale, M. & Valle, F., 2022 feb. 1, I: Colloids and Surfaces B: Biointerfaces. 210, 112231.
32. **Nanoscale Structure and Dynamics of Model Membrane Lipid Raft Systems, Studied by Neutron Scattering Methods.** Ahmadi, D., Thompson, K. C., García Sakai, V., Schweins, R., Moulin, M., Haertlein, M., Strohmeier, G. A., Pichler, H., Forsyth, V. T., Barlow, D. J., Lawrence, M. J. & Foglia, F., 2022 apr. 27, I: Frontiers in Physics. 10, 864746.
33. **Nanostructurally Controllable Strong Wood Aerogel toward Efficient Thermal Insulation.** Garemark, J., Perea-Buceta, J. E., Rico Del Cerro, D., Hall, S., Berke, B., Kilpeläinen, I., Berglund, L. A. & Li, Y., 2022 juni 1, I: ACS Applied Materials and Interfaces. 14, 21, s. 24697-24707 11 s.

34. **Neutron crystallography reveals mechanisms used by *Pseudomonas aeruginosa* for host-cell binding.** Gajdos, L., Blakeley, M. P., Haertlein, M., Forsyth, V. T., Devos, J. M. & Imberty, A., 2022, I: Nature Communications. 13, 1, 194.
35. **Parkinson's disease and multiple system atrophy patient iPSC-derived oligodendrocytes exhibit alpha-synuclein-induced changes in maturation and immune reactive properties.** Azevedo, C., Teku, G., Pomeschchik, Y., Reyes, J. F., Chumarina, M., Russ, K., Savchenko, E., Hammarberg, A., Lamas, N. J., Collin, A., Gouras, G. K., Klementieva, O., Hallbeck, M., Taipa, R., Vihinen, M. & Roybon, L., 2022, I: Proceedings of the National Academy of Sciences of the United States of America. 119, 12, e2111405119.
36. **Polymer-Mediated Interactions and Phase Behaviour of Polymer-Particle Dispersions.** Haddadi, S., 2022 apr. 28, Lund University. 139 s.
37. **Prolonged heat and drought versus cool climate on the Swedish spring wheat breeding lines: Impact on the gluten protein quality and grain microstructure.** Lama, S., Vallenback, P., Hall, S. A., Kuzmenkova, M. & Kuktaite, R., 2022, I: Food and Energy Security. 11, 2
38. **Quantifying the hierarchy of structural and mechanical length scales in granular systems.** Shahin, G., Herbold, E. B., Hall, S. A. & Hurley, R. C., 2022 feb., I: Extreme Mechanics Letters. 51, 101590.
39. **Self-Interactions of Two Monoclonal Antibodies: Small-Angle X-ray Scattering, Light Scattering, and Coarse-Grained Modeling.** Mahapatra, S., Polimeni, M., Gentiluomo, L., Roessner, D., Frieß, W., Peters, G. H. J., Streicher, W. W., Lund, M. & Harris, P., 2022, I: Molecular Pharmaceutics. 19, 2, s. 508-519
40. **Shape Matters in Magnetic-Field-Assisted Assembly of Prolate Colloids.** Pal, A., De Filippo, C. A., Ito, T., Kamal, M. A., Petukhov, A. V., De Michele, C. & Schurtenberger, P., 2022 feb. 22, I: ACS Nano. 16, 2, s. 2558-2568 11 s.
41. **Shining infrared light on amyloid structures in neurodegenerative proteinopathies.** Paulus, A., 2022, Lund: Lund University, Faculty of Medicine. 78 s.
42. **Structure and anisotropic dynamics of stimuli responsive colloidal ellipsoids at the nearest neighbor length scale.** Pal, A., Kamal, M. A. & Schurtenberger, P., 2022, I: Journal of Colloid and Interface Science. 621, s. 352-359 8 s.
43. **The Influence of pH on the Lipase Digestion of Nanosized Triolein, Diolein and Monoolein films.** Humphreys, B. A., Campos-Terán, J., Arnold, T., Baunsgaard, L., Vind, J., Dicko, C. & Nylander, T., 2022, I: Frontiers in Soft Matter. 2, 13 s., 929104.
44. **The scale of a martian hydrothermal system explored using combined neutron and x-ray tomography.** Martell, J., Alwmark, C., Daly, L., Hall, S., Alwmark, S., Woracek, R., Hektor, J., Helfen, L., Tengattini, A. & Lee, M., 2022 maj 11, I: Science Advances. 8, 19, 3044.
45. **The synaptic and neurobiological role of apolipoprotein E4 in models of Alzheimer's disease.** Konings, S., 2022, Lund: Lund University, Faculty of Medicine. 108 s.
46. **Towards a multiconfigurational description of the electronic structure in solids.** Larsson, E. D., 2022 okt. 31, Lund: Lunds Universitet/Lunds Tekniska Högskola. 101 s

47. **Recommendations for Addressing the Translational Gap between Experimental and Clinical Research on Amyloid Diseases.** Miriam Solomon; Vito Foderà; Annette Eva Langkilde; Perry Elliott; Fabrizio Tagliavini; Trevor Forsyth; Oxana Klementieva; Vittorio Bellotti. *Journal of Translational Medicine*, 13 May 2022.
48. **On the extension of a physical body in classical motion. An analogy between a pseudo-velocity concept and Wiener's process in (ideal) polymer solutions.** Stefano A. Mezzasalma, *Results in Physics*, Volume 34, March 2022.
49. **Aquaglyceroporins and orthodox aquaporins in human adipocytes.** Huang P, Hansen JS, Saba KH, Bergman A, Negoita F, Gourdon P, Hagström-Andersson A, Lindkvist-Petersson K. *Biochim Biophys Acta Biomembr.* 2022 Feb 1.
50. **Analyses of the complex formation of Staphylococcal Enterotoxin A and human gp130 cytokine receptor.** Sibel Uzunçayır, Arturo Vera-Rodriguez, Paulina Regenthal, Hannah Åbacka, Cecilia Emanuelsson, Christopher D. Bahl, Karin Lindkvist-Petersson. *FEBS Lett.* 2022 Jan 21. Online ahead of print.
51. **Self-Diffusive Properties of the Intrinsically Disordered Protein Histatin 5 and the Impact of Crowding Thereon: A Combined Neutron Spectroscopy and Molecular Dynamics Simulation Study.** Eric Fagerberg, Samuel Lenton, Tommy Nylander, Tilo Seydel, and Marie Skepö. 2022 Jan 19. *Journal of Physical Chemistry.*
52. **Neutron crystallography reveals mechanisms used by *Pseudomonas aeruginosa* for host-cell binding.** Lukas Gajdos, Matthew P Blakeley, Michael Haertlein, Trevor Forsyth, Juliette M Devos, Anne Imberty, 2022 Jan 11. *Nature Communications.*
53. **Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction.** Victoria N. Drago, Juliette M. Devos, Matthew P. Blakeley, V. Trevor Forsyth, Andrey Y. Kovalevsky, Constance A. Schall & Timothy C. Mueser, 2022: *npj Microgravity* volume 8, Article number: 13
54. **Untangling the threads of cellulose mercerization.** Daisuke Sawada, Yoshiharu Nishiyama, Riddhi Shah, V. Trevor Forsyth, Estelle Mossou, Hugh Michael O'Neill, Masahisa Wada, Paul Langan, 2022: *Nature Communications* volume 13, Article number: 6189 (2022)

Reported by the New Materials Theme (without formal affiliation)

1. Report on the Workshop on "Magnetic Small Angle Neutron Scattering - Data Analysis and Software Prospects", Annika Stelhorn, Wojciech Potrzebowski & Paul D. Butler, (2022) *Neutron News*, 33:4, 9-10.
2. Emma Campillo, *Supraledning vid starka magnetfält*, *Fysikaktuellt* 4, p. 22, December 2022. Publication resulting from *Fysikdagarna 2022 (LINXS-related Event)* – poster prize winner was affiliated with LINXS, and the prize was a (popular science) article in the magazine of the Swedish Physical Society
3. Emma Campillo, Maciej Bartkowiak, Oleksandr Prokhnenko, Peter Smeibidl, Edward Forgan and Elizabeth Blackburn, *Analysis of time-of-flight small-angle neutron scattering data on mesoscopic crystals such as magnetic vortex lattices.* *J. Appl. Cryst.* **55**, 1314 (2022) – doi:10.1107/51600576722008226
4. A part of a virtual special issue on Magnetic SANS organised by a group including some LINXS Fellows and published February 2023 (fellows involved: Andreas Michels,

Sebastian Muehlbauer, Elliot Paul Gilbert) ([\(IUCr\) Magnetic small-angle neutron scattering \$\hat{a}\$ " from nanoscale magnetism to long-range magnetic structures](#))

Reported by the ISB and IPDD Themes (without formal affiliation)

5. Microfluidic-Derived Detection of Protein-Facilitated Copper Flux Across Lipid Membranes. Górecki K, Hansen JS, Li P, Nayeri N, Lindkvist-Petersson K, Gourdon P. *Anal Chem.* 2022 Aug 30;94(34):11831-11837.
6. Structures of Atm1 provide insight into [2Fe-2S] cluster export from mitochondria. Li P, Hendricks AL, Wang Y, Villones RLE, Lindkvist-Petersson K, Meloni G, Cowan JA, Wang K, Gourdon P. *Nat Commun.* 2022 Jul 27;13(1):4339.
7. PcoB is a defense outer membrane protein that facilitates cellular uptake of copper. Li P, Nayeri N, Górecki K, Becares ER, Wang K, Mahato DR, Andersson M, Abeyrathna SS, Lindkvist-Petersson K, Meloni G, Missel JW, Gourdon P., *Protein Sci.* 2022 Jul;31(7):e4364.
8. Small-molecule activation of OGG1 increases oxidative DNA damage repair by gaining a new function. Michel M, Benítez-Buelga C, Calvo PA, Hanna BMF, Mortusewicz O, Masuyer G, Davies J, Wallner O, Sanjiv K, Albers JJ, Castañeda-Zegarra S, Jemth AS, Visnes T, Sastre-Perona A, Danda AN, Homan EJ, Marimuthu K, Zhenjun Z, Chi CN, Sarno A, Wiita E, von Nicolai C, Komor AJ, Rajagopal V, Müller S, Hank EC, Varga M, Scaletti ER, Pandey M, Karsten S, Haslene-Hox H, Loevenich S, Marttila P, Rasti A, Mamonov K, Ortis F, Schömberg F, Loseva O, Stewart J, D'Arcy-Evans N, Koolmeister T, Henriksson M, Michel D, de Ory A, Acero L, Calvete O, Scobie M, Hertweck C, Vilotijevic I, Kalderén C, Osorio A, Perona R, Stolz A, Stenmark P, Berglund UW, de Vega M, Helleday T. *Science.* 2022 Jun 24;376(6600):1471-1476.
9. Nudix hydrolase 18 catalyzes the hydrolysis of active triphosphate metabolites of the antivirals remdesivir, ribavirin, and molnupiravir. Jemth AS, Scaletti ER, Homan E, Stenmark P, Helleday T, Michel M. *J Biol Chem.* 2022 Aug;298(8):102169.
10. The First Structure of Human MTHFD2L and Its Implications for the Development of Isoform-Selective Inhibitors. Scaletti ER, Gustafsson Westergren R, Andersson Y, Wiita E, Henriksson M, Homan EJ, Jemth AS, Helleday T, Stenmark P. *ChemMedChem.* 2022 Sep 16;17(18):e202200274.
11. Pharmacological targeting of MTHFD2 suppresses acute myeloid leukemia by inducing thymidine depletion and replication stress. Bonagas N, Gustafsson NMS, Henriksson M, Marttila P, Gustafsson R, Wiita E, Borhade S, Green AC, Vallin KSA, Sarno A, Svensson R, Göktürk C, Pham T, Jemth AS, Loseva O, Cookson V, Kiweler N, Sandberg L, Rasti A, Unterlass JE, Haraldsson M, Andersson Y, Scaletti ER, Bengtsson C, Paulin CBJ, Sanjiv K, Abdurakhmanov E, Pudelko L, Kunz B, Desroses M, Iliev P, Färnegårdh K, Krämer A, Garg N, Michel M, Häggblad S, Jarvius M, Kalderén C, Jensen AB, Almlöf I, Karsten S, Zhang SM, Häggblad M, Eriksson A, Liu J, Glinghammar B, Nekhotiaeva N, Klingegård F, Koolmeister T, Martens U, Llona-Minguez S, Moulson R, Nordström H, Parrow V, Dahllund L, Sjöberg B, Vargas IL, Vo DD, Wannberg J, Knapp S, Krokan HE, Arvidsson PI, Scobie M, Meiser J, Stenmark P, Berglund UW, Homan EJ, Helleday T. *Nat Cancer.* 2022 Feb;3(2):156-172.

12. Sialic acid derivatives inhibit SiaT symporters and attenuate bacterial growth. T. Bozzola, C. Rovegno, M. F. Scalise, A. Mitra, J. Cramer, R. Johnsson, J. Schelin, C. Indiveri, R. Friemann, U. J. Nilsson, U. Ellervik. *ACS Chem. Biol.*, Article ASAP, 2022.
13. Discovery and Optimization of the First Highly Effective and Orally Available Galectin-3 Inhibitors for Treatment of Fibrotic Disease. F. Zetterberg, A. McKinnon, T. Brimert, L. Gravelle, R. Johnsson, B. Kahl-Knutsson, H. Leffler, U. J. Nilsson, A. Pedersen, K. Peterson, J. Roper, H. Schambye, R. Slack, S. Tantawi. *J. Med. Chem.*, 2022, 65, 12626-12638. Featured as a "Molecule of the Month" by Drug Hunter in September 2022.
14. Design and synthesis of novel 3-triazolylgalactosides as galectin-1, -3 and -8 inhibitors S. van Klaveren, J. Dernovšek, Ž. Jakopin, M. Anderluh, H. Leffler, U. J. Nilsson, and T. Tomašič. *RSC Adv.*, 2022, 12, 18973-18984.
15. Sialic acid 4-N-piperazine and piperidine derivatives target sialic acid uptake by the *P. mirabilis* sodium solute symporter. T. Bozzola, R. Johnsson, U. J. Nilsson, and U. Ellervik *ChemMedChem*, accepted, 2022.
16. Sirtuin 1-Activating Compounds: Discovery of a Class of Thiazole-Based Derivatives Bononi, G., Citi, V., Lapillo, M., Martelli, A., Poli, G., Tuccinardi, T., Granchi, C., Testai, L., Calderone, V., Minutolo, F. *Molecules*, 2022, 27 (19), art. no. 6535.
17. Reversible Monoacylglycerol Lipase Inhibitors: Discovery of a New Class of Benzylpiperidine Derivatives. Bononi, G., Di Stefano, M., Poli, G., Ortore, G., Meier, P., Masetto, F., Caligiuri, I., Rizzolio, F., MacChia, M., Chicca, A., Avan, A., Giovannetti, E., Vagaggini, C., Brai, A., Dreassi, E., Valoti, M., Minutolo, F., Granchi, C., Gertsch, J., Tuccinardi, T. *Journal of Medicinal Chemistry*, 2022, 65 (10), pp. 7118-7140.
18. New Synthetic Analogues of Natural Polyphenols as Sirtuin 1-Activating Compounds Bononi, G., Flori, L., Citi, V., Acciai, C., Nocilla, V., Martelli, A., Poli, G., Tuccinardi, T., Granchi, C., Testai, L., Calderone, V., Minutolo, F. *Pharmaceuticals*, 2022, 15 (3), art. no. 339.
19. The effect of lactate dehydrogenase-A inhibition on intracellular nucleotides and mitochondrial respiration in pancreatic cancer cells. Franczak, M., Kutryb-Zajac, B., El Hassouni, B., Giovannetti, E., Granchi, C., Minutolo, F., Smolenski, R.T., Peters, G.J. *Nucleosides, Nucleotides and Nucleic Acids*, 2022, 41:12, 1375-1385.
20. New PIN1 inhibitors identified through a pharmacophore-driven, hierarchical consensus docking strategy. Poli, G., Di Stefano, M., Estevez, J.A., Minutolo, F., Granchi, C., Giordano, A., Parisi, S., Mauceri, M., Canzonieri, V., Macchia, M., Caligiuri, I., Tuccinardi, T., Rizzolio, F. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, 37 (1), pp. 145-150.
21. MAGL inhibitor NanoMicellar formulation (MAGL-NanoMicellar) for the development of an antiglaucoma eye drop. Chetoni, P., Burgalassi, S., Zucchetti, E., Granchi, C., Minutolo, F., Tampucci, S., Monti, D. *International Journal of Pharmaceutics*, 2022, 625, art. no. 122078.

Annex 4 – LINXS Community 2022

In 2022, LINXS Fellows came from the following organisations:

1. Aarhus University, Denmark
2. Alfa Laval Sweden
3. Arla Foods, Sweden
4. Arwa Foodtech AB, Sweden
5. AstraZeneca Mölndal, Sweden
6. Australian Synchrotron (ANSTO), Australia
7. Centro de Física de Materiales (CSIC-UPV/EHU), Spain
8. Chalmers University of Technology, Sweden
9. Deutsches Elektronen-Synchrotron DESY, Germany
10. European Molecular Biology Laboratory (EMBL) Hamburg, Germany
11. European Spallation Source ESS AB, Sweden
12. Forschungszentrum Juelich GmbH, Germany
13. French Institute of Health and Medical Research, France
14. Fritz Haber Institute Berlin, Germany
15. Hamburg University, Germany
16. Institut de Biologie Structurale (IBS) - Grenoble, France
17. ICREA, Catalan Institute of Nanoscience and Nanotechnology, Spain
18. ISIS Facility, STFC, United Kingdom
19. Johnson Matthey Formox AB, Sweden
20. Karlstad University, Sweden
21. Karolinska Institutet, Sweden
22. KTH Royal Institute of Technology, Sweden
23. La Trobe University, Australia
24. Linnaeus University, Sweden
25. Lund University, Sweden
26. Malmö University, Sweden
27. MAX IV, Sweden
28. Novartis, Switzerland
29. Norwegian University of Science and Technology, Norway
30. Novo Nordisk, Denmark
31. Novozymes, Lyngby, Denmark
32. Oatly, Sweden
33. Örebro Universitet, Sweden
34. Pfizer, USA
35. Research institutes of Sweden (RISE), Sweden
36. RWTH Aachen University, Germany
37. Spanish Council for Scientific Research (CSIC), Spain
38. Stockholm University, Sweden
39. Swedish University of Agricultural Sciences (SLU), Sweden
40. Tampere University, Finland
41. Technical University of Darmstadt (TU Darmstadt), Germany
42. Technical University of Munich (TUM), Germany
43. Technical University of Denmark (DTU), Denmark

44. Tetra Pak, Sweden
45. University of Copenhagen, Denmark
46. University of Florida, USA
47. University of Gothenburg, Sweden
48. Université Grenoble Alpes, France
49. University of Helsinki, Finland
50. University of Luxemburg, Luxemburg
51. University of Newcastle, United Kingdom
52. University of Nottingham, United Kingdom
53. University of Pavia/University College London, United Kingdom
54. University of Pisa, Italy
55. University of Regensburg, Germany
56. University of Santiago de Compostela, Spain
57. University of Southern Denmark, Denmark
58. Uppsala University, Sweden

Annex 5 – Financial reporting 2022

Income statement	Categories	Description	SEK
Income	Activities	Conference fees	380,927
	Activities Total		380,927
	Partners contribution	LTH funding	2,000,000
		LU Central funding	2,500,000
		MedFak funding*	1,000,000
		N-Fak funding	3,000,000
	Partners contribution Total		8,500,000
	Membership fees	Membership RISE	50,000
	Membership fees Total		50,000
	External funding	Deferral **	-5,834,435
		LMK Foundation	1,000,000
		SAGA GISANS	6,379,152
		Sponsoring	5,000
External funding Total		1,549,717	
Income Total		10,480,644	
Expenditure	Activities	Conference cost	-695,281
		Hotel & housing	-254,293
		Participation conferences	-59,679
		Representation external	-59,904
		Travel	-348,597
	Activities Total		-1,417,755
	Equipment/furniture	Deprecation	-76,402
	Equipment Total		-76,402
	Materials & consumables	Computer/Screen/Electronics	-101,086
		Office supply	-73,030
		Other (currency exchange)	-26,127
		Print material	-35,899
		Services/Maintenance	-63,453
	Materials & consumables Total		-299,595
	Overhead	OH	-1,645,116
	OH Total		-1,645,116
	Premises	Cleaning	-104,808
Premises		-1,130,850	
Premises Total		-1,235,658	
Salaries	LMK Foundation	-275,702	
	SAGA GISANS	-744,166	
	Salaries	-4,042,832	
Salaries Total		-5,062,700	
Expenditure Total		-9,737,226	
Total result 2022		743,418	

* In addition, the Lund University faculty of Medicine contributed in-kind with 20% of the salary of the LINXS co-director and of that of the IPDD Theme leader.

** Deferral of SAGA GISANS, LMK, FORMAS projects funding implemented in 2022 towards 2023.

Annex 6 – Highlights and Legacy 2022

Highlights – New Materials Theme

➤ **Magnetic SANS and SasView**

Link to original article, published Jun 20st, 2022 in SasView for Small Angle Scattering Analysis website: <https://www.sasview.org/2022-06-20-LINXS-workshop/>

On June 13-14, 2022, LINXS held a hybrid Magnetic SANS Workshop in Lund. Over the course of the Workshop some of the current research in the area, spanning diffraction to diffuse scattering, were presented and the software tools required to simplify the data analysis task were discussed. The SasView team presented its concept of an “open collaborative community-driven development” approach and the advantages this brings, along with recent developments targeted at the Magnetic SANS community. There was a feeling that the new developments in SasView were already quite useful and that there is potential for some further contributions. The community-driven concept was greatly appreciated by the workshop participants who enthusiastically suggested ideas for new workflows, model functions, meta-data storage, etc.

The LINXS workshop was immediately followed by a 3 day in-person Contributor Training Workshop/Hackathon in which a few of the LINXS participants, along with a couple of other new contributors, learned some of the basics of contributing to the project and used this knowledge to work on real projects.

It was quite exciting to see the old “Code Camp” dynamic back in play and we look forward now to the resumption of Code Camps and to working to empower the broader community to contribute to SasView.

➤ **The Catalysis Working Group has Established New Collaborations and Stimulated Ongoing Projects**

Link to original article, published Jun 20st, 2022 in the LINXS website: <https://www.linxs.se/news/2022/12/12/the-catalysis-working-group-established-new-collaborations-and-stimulated-already-ongoing-projects>

The Catalysis working group has been in existence for two years. Sara Blomberg, Associate Senior lecturer at the Department of Chemical Engineering at Lund University, and working group leader, is happy with how the work is progressing: – We have established new collaborations but also stimulated already ongoing joint projects.

The Catalysis working group aims to increase fundamental knowledge and understanding on catalysis. The group strives to facilitate collaboration and create arenas for new scientific discoveries. Since the group was formed, under the New Materials Theme, it has organised two workshops to gather different researchers in the field.

The most recent event in June, which gathered 30 participants, focused on X-ray based research related to catalysis theory and electrochemistry. Both experimentalists and

theoreticians attended the workshop. Sara Blomberg notes that it is good to present many different perspectives, so that you can gain more in-depth knowledge of the area.

– We want these events to be informal to help with networking, and to spark new research discussions. They also present an opportunity to invite senior scientists to come and present, and for younger PhDs to talk about their science. I think this is very important in terms of younger researcher gaining new contacts and ideas.

LINXS Guest researcher programme is beneficial for collaborations.

She is very pleased with the overall progress of the group's work. Inviting visiting guest researcher Jason Weaver, Professor in Chemical Engineering, from Florida University, in the USA, has been very fruitful. He stayed at LINXS from May unto July 2022. She says that having someone stay for a longer period, which is the aim of LINXS visiting guest researcher programme, is important in terms of enabling more focused discussions – which in this case led on to formal collaborations in the form of beamtime proposals.

– We have been able to send in several joint proposals for beamtime at different synchrotrons. The joint beamtime applications is another result of the large network created within our group where people bring in colleagues from their home universities.

The beamtime proposals focuses on situ-experiments with an aim to increase the fundamental understanding of catalysis and cover both electrochemistry and thermal catalysis. Questions that are important to investigate include for example, how do catalyst materials behave in gases or in other chemical processes? And what happen to the catalysis process when you change the material alloy, or change its properties?

Bridge the gap between industry and fundamental science.

Sara Blomberg explains that the proposals bring together people who work on both applied and fundamental catalysis.

– Since I work a lot with industry, I hope that our experiments can prove useful for them too. One goal with our working group is to bridge the gap between industry and fundamental science. Therefore, we want to involve industry and get their input too. The overall aim is of course to have more efficient catalysis: but how should the process look like: how should we get there? Industry can help guide us scientists in terms of what questions we should ask, and how we should design our experiments to mimic industrial conditions, she concludes.

Highlights – Northern Lights on Food Theme (NLF)

- **Northern Lights on Food Conference III, from milk to limoncello – The best of food science and innovation**

Link to original article, published in the LINXS website Jun 29th, 2022:

<https://www.linxs.se/news/2022/6/29/northern-lights-on-food-conference-iii-from-milk-to-limoncello-the-best-of-food-science-and-innovation>

Northern Lights on Food III was the third annual conference bringing together researchers from academia and industry. Three days of presentations included new research using x-ray and neutron tools to make progress in our understanding of food structures, as well as connections to the wider food industry and society as a whole. After last year's conference was an online-only event, this year 80 participants gathered in the heart of Lund to meet once more in person, learn about each other's work, and discuss the way forward for the Northern Lights on Food initiative.

The opening keynote presentation was given by Prof. Elliot Gilbert from ANSTO Australia, who provided a comprehensive summary of how scattering can be used in the characterisation of food materials. The focus was starch, where Prof. Gilbert has made significant contributions to the structural analyses of different types of starches, and how these structures are affected by food processing.

"It is fantastic to finally meet people again after two years, and especially to discuss this fascinating topic. The development of food materials requires interdisciplinary research, and Northern Lights on Food offers this: to let researchers from diverse backgrounds to come together. And in such an engaging and friendly environment, Prof. Gilbert says.

From there, the first two days of the conference featured a wide array of subjects and participants. This included talks on cellulose in plant-based foods, the structure and function of lipid systems, and several examples of food processing and direct applications. Day two included a session on industrial access to large-scale facilities, as well as broader talks on changing consumer behaviour, and assessing social and environmental impacts of food production using a systems perspective. Hanna Barriga from Karolinska Institutet summarize:

"The NLF conference is an excellent platform for industrial and academic partners to share data, discuss projects and identify the challenges within the sector that we can contribute to. It really encompassed the NLF ethos of working together to provide solutions using scattering techniques."

Day three of the workshop focused on strategy discussions – how to build up the collaboration platform for future food solutions. Prof. Daniel Söderberg (KTH, Director of Treesearch) was invited to describe the establishment of the Treesearch platform, and the lessons learnt along the way. Prof. Rickard Öste (founder of Oatly) also summarized the need to create new knowledge in food material science.

The discussion that followed led to the clarification of the general aims of Northern Lights on Food:

- To focus on solvable research questions that can make a real difference to today's food systems.
- To create an environment that attracts young scientists and students to the world of food science and research.
- To bridge the communicative gap between food scientists and the facilities.

Finally, the discussion group agreed on some actions. During the upcoming months, the Northern Lights on Food platform will decide on a vision, identify all complimentary techniques available, develop and strengthen the masterclasses offered, and define a way forward through long term funding opportunities.

➤ **Food Colloids Workshop Identified Common Challenges Related to the Use Of X-Ray and Neutron Scattering Techniques in Food**

Link to original article, published in the LINXS website Dec 13th, 2022:

<https://www.linxs.se/news/2022/12/2/food-colloids-workshop-identified-common-challenges-related-the-use-of-x-ray-and-neutron-scattering-techniques>

Around 40 people attended in October the hybrid Industry Workshop on Food Colloids and Structured Interfaces co-organised by Ben Boyd, Professor at the Department of Pharmacy, University of Copenhagen, Associate Professor Jacob Kirkensgaard from Department of Food Science, University of Copenhagen, and Dr Ulf Andersen from Arla Foods. The event aimed to facilitate networking between companies, provide an arena to exchange ideas, and identify common challenges in relation to food and the use of X-ray and neutron scattering techniques.

Ben, a member of the Northern Lights on Food, Working Group on Food Colloids and Structured Interfaces, reflects that the workshop went well.

– The whole intention of the event was to get companies to talk with each other, and discuss what they are doing and how they are using scattering approaches to solve problems. This is an important aspect since many companies face similar issues. It is also a way of inspiring each other, and increase knowledge on how, and when, to use scattering techniques to gain knowledge about food structures.

Common challenges were identified.

So what challenges are common for industry? According to Ben they centre on lack of knowledge of who talk to at large scale facilities, and an uncertainty of what problems scattering techniques can help to solve. Another question is at what point one should take a problem or query to a large-scale facility.

– It was good to discuss these issues and point to solutions. One specific outcome is reinforcing that that scattering is not generally a kind of imaging technique which is often a misconception. But I think the industry cases we presented gave a good idea of the great possibilities afforded by X-ray and neutron scattering.

– We also discussed the importance of industry having a dialogue with people working at lab scale, maybe at universities or institutes, as soon as a research question arises. These people can advise on whether the problem needs to be investigated using a lab source which can be simpler and easier to access than the large-scale facilities. One has to remember that it can be quite hard to get access to larger facilities, and that much experience and knowledge are required to perform experiments.

Important to have places like LINXS to act as a conduit in linking industry to facilities.

Ben goes on to say that these types of events are important to increase capacity and understanding amongst industry on how to think about scattering experiments. Places like LINXS and the Danish Technological Institute are also invaluable in acting as conduits in linking industry scientists to people working at large scale facilities.

What does he believe will be the next frontier in food science? He is quick to answer: food efficiency and nutrition value. Producing food that is high in nutrients, healthy and do not contribute negatively to greenhouse gas emissions will be paramount to feed a growing population. To produce this type of food more knowledge on what happens to the food in the gut is needed – his own area of research is in structure of food during digestion.

– There is much that we are still learning about digestion and structure and their impact on the performance of food. That excites me. With my background in the pharmaceutical industry, I am very interested in what happens to foods structures as the components are broken down, and how that in turn affects delivery and absorption of nutrients.

More attention is needed on what happens with food after it is digested.

In his own research, he has used X-ray and neutron scattering to investigate the breakdown of milk fats which is key to delivery of lipids and poorly soluble nutrients. His experiments have shown that milk fat droplets form many structures, which interact with other components in milk to modify digestion and delivery. These results could be important for the development of non-dairy drink alternatives which sets out to mimic the nutritional benefits of milk.

– In coming years, I would like to see way more attention on what happens to food after it is digested. Developing this, largely unknown, research field will be really crucial, I believe if we want to ensure food security, and also maintaining our health. Practical ways of doing this, could for example be to use scattering techniques to study not only food structure but also the way in which food particles interact with gut biology such as cells and instinal surfaces or mucus, for example, he concludes.

➤ **Guest Researcher Elliot Gilbert Reflects on Food, Health and Getting Ready for ESS**

Link to original article, published in the LINXS website Sep 5th, 2022:

<https://www.linxs.se/news/2022/9/5/nlf-guest-researcher-elliott-gilbert-reflects-on-food-health-and-getting-ready-for-ess>

During the summer, Professor Elliot Gilbert, Leader of Food Materials Science, and instrument scientist at the Australian Nuclear Science and Technology Organisation, spent time at LINXS as part of the institute's guest researcher programme. He was invited by the Northern Lights on Food Theme.

In the context of the Theme, his expertise lies in the application of advanced characterization techniques including neutrons and X-ray scattering for studying food materials, as well as the development of specialized sample environments. In the field of starch, he has made significant contributions to the structural analyses of different types of starches, and how these structures are affected by food processing.

– What is happening within the Theme is really exciting. The approach is similar to how we at ANSTO developed a community around using large scale infrastructures to gain new knowledge on food materials more than 15 years ago.

– I am particularly impressed with the network that has already been established and the significant number of industrial partners that are involved. This is enormously encouraging.

Communicating the value of using large scale infrastructure.

It's still a huge challenge, according to Elliot Gilbert, to communicate and demonstrate the value of using large scale infrastructure to industry researchers, even though neutron and X-ray techniques can play a crucial role in the development of new products and processes, especially in terms of designing alternative protein sources that can feed a growing population, while also reducing the negative climate impacts of food production. Foods that can improve human health are also greatly needed. One such example are starch products that are less digestible, enabling gut friendly bacteria to be supported in the large intestine. These bacteria have been shown to produce chemicals that cause cell death in colon cancer, one of the leading causes of cancer death.

He emphasises that initiatives such as the Northern Lights on Food Theme can play a significant part in enabling the huge leaps that society needs to transform how we produce and consume food.

– An important goal, as I see it, not just for the Theme and LINXS, but for all of us that work with large scale research infrastructures, is to highlight the difference they can make. Their role is to provide knowledge and guidance on the interplay between structure, function and processing - results that can then be used by the food industry, and other researchers, to innovate.

Getting ready for ESS needs to be a priority.

Reflecting further, he adds that it is paramount that the Theme, and the broader neutron community, in parallel with communicating with the food industry, also focuses on getting ready to make use of ESS at the earliest opportunity. ESS is set to become fully operational by 2027.

– You are entering a very unique time here in the South of Sweden, where you have both access the MAX IV synchrotron, and soon one of the world's most intense neutron sources.

– At ANSTO, we are happy to help in the development of your local neutron community in how to get the best out of these new facilities. As the only nuclear facility with a dedicated programme in food materials, we can offer a range of support including advice to potential users, consultations with stakeholders, as well as actual neutron experiments and specialized sample environments.

Elliot Gilbert is looking forward to following the Theme and the broader community's progression over the next couple of years:

– I had a very a rewarding stay at LINXS, both personally and professionally. I can see many areas where we at ANSTO can actively engage and numerous opportunities for greater collaboration within food science in the future.

Highlights – Integrative Pharmacology and Drug Discovery Theme (IPDD)

- **IPDD Kicked off and all Work Groups are Active**

Link to original article, published in the LINXS website May 15th, 2022:

<https://www.linxs.se/news/2022/6/20/ipdd-kicked-off-and-all-work-groups-are-active>

The new Theme for Integrative Pharmacology and Drug Discovery (IPDD) gathered many members at the kick-off in April, both from the national community and from abroad. The working groups have different approaches and complement each other in interesting ways around drug discovery and development.

Karin Lindkvist, Theme leader was very happy with the turnout and the discussions at the event:

“To start with, we were of course very glad to meet in person and have talks face-to-face. The level of engagement was also great, and we realised that we can learn a lot from our various backgrounds, although it can also be a bit of a challenge”.

A central idea is that the working groups will invite each other to seminars, workshops and similar so there can be a knowledge transfer and bridge between fields.

“There is a lot in the area of Biomedical Imaging that is new to me, says Karin Lindkvist. It is fantastic to see what can be done and it would be extremely valuable to have a beamline for this also at MAX IV in Lund. Now this research must be carried out elsewhere, like Grenoble”.

There are not many researchers in Sweden who are active in the area of Structure-based drug design, in which Karin Lindkvist is active herself. She sees a chance to maybe strengthen the topic nationally and also learn from fellow researchers in Denmark where the field is much stronger.

“Here, there is more research and development carried out by industry, rather than in academia. However, their focus is on mainly finding promising new drugs whereas we can develop methodologies and test new technologies”, says Karin Lindkvist.

Just as many other researchers, Karin Lindkvist is actively engaged in dialogues with smaller biotech companies that can develop research results to commercial solutions. This provides both parties with opportunities to learn and transfer knowledge which is beneficial to all.

Some events have already launched and there are more planned for after the summer break. A proposal from the kick-off was also to find out if yet another working group could be set up, targeting Drug delivery. An internal workshop will take place probably in late August to gather interest from those who can engage in this area.

➤ **Workshop has Set the Scene for “Biomedical Imaging for Drug Discovery and Development” and Started Important Dialogues**

Link to original article, published in the LINXS website Dec 13th, 2022:

<https://www.linxs.se/news/2022/12/12/workshop-set-the-scene-for-biomedical-imaging-for-drug-discovery-and-development-and-started-important-dialogues>

Up to now synchrotron techniques have rarely been used in the latter stages of biomedical drug development and drug discovery processes. A novel educational workshop, organised

by the Biomedical Imaging working group, as part of LINXS' IPDD Theme, gathered 40 participants in mid-October, with another 23 people attending online.

– I see the use of synchrotron imaging as a method to turn to when you get stuck during a drug discovery and development process. To be able to see what is happening in high resolution during experiments with live animals can potentially add that extra bit of information you need, says Lars E. Olsson, Professor of Medical Physics at Lund University, and working group leader.

Processes, hurdles, and development of new drugs explained.

During the workshop, scientists from the pharmaceutical industry explained the process and the hurdles in drug discovery and development, and how biomedical imaging can be used to facilitate the process. Educational lectures were also given, which reviewed the imaging methods for both synchrotron imaging and competing imaging technologies. In addition, state-of-the-art lectures on biomedical imaging applications from the synchrotron facilities at ESRF and PSI, were also presented.

In the panel debate that followed, the focus was on how biomedical imaging can be developed at MAX IV. The main topics were "ECO-system", i.e. how do we bring researchers together from different disciplines for applications at MAX IV? Further, it was discussed that the many, but scattered initiatives, to promote in-vivo imaging are suboptimal to promote the MedMAX beamline. In addition, the need for practical help to users with data handling and analysis were expressed.

– It is important to concentrate efforts, and gather these scattered initiatives, as well as look into ways to support researchers looking to use X-rays. One aspect of that is getting networks and contacts together so that we are ready once MedMAX opens. The field of drug discovery is moving very fast, and here we have techniques that can yield novel information.

Lars E Olsson, reflects that he is happy with the workshop:

– It was very well received, and it set the scene for progress on "Biomedical Imaging for drug discovery and development". During the day, we started dialogues that will be bring scientists together on future in-vivo drug applications at MAX IV, he says.

The seminars from the workshop are recorded and are available on the LINXS Educational page.

➤ **Meeting on Structure Based Drug Design Provided a Good Opportunity to Build National Networks**

Link to original article, published in the LINXS website Jan 25th, 2023:

<https://www.linxs.se/news/2023/1/25/meeting-on-drug-design-provided-a-good-opportunity-to-build-networks-nationally>

In mid-November, the Structure-based Drug Design working group, within the IPDD Theme, invited researchers to a meeting on structure-based drug design. The ambition was to gather researchers working on different aspects of structure-based drug design and to build a

network of researchers wishing to use X-ray and neutron techniques to develop new drugs. Around 40 people attended the two-day event.

– The general feeling was that people enjoyed the meeting. The atmosphere was nice and open. We had lots of interaction and discussions in the coffee break, says Raminta Venskutonyte, Assistant researcher at Medical Structural Biology, Lund University, and working group leader.

She reflects that most participants were from Swedish universities, and that the meeting provided a good opportunity to establish networks nationally.

– For example, I had no idea that there is a group of researchers working with structure-based drug design in Gothenburg. It is great that our groups have now established contact, especially since they focus on the computational aspects of drug design, which we do not. It was also good to inform people about LINXS, which is not so known to some researchers yet.

The programme was divided into four sessions and covered topics such as fragment-based drug discovery and potential drug compound binding mode studies using computational methods, PROTAC technology, structural studies of medically relevant membrane proteins using X-ray crystallography and cryoEM, which provide strategies for future drug development.

Next steps - a PhD course and follow up meeting.

The next step for the Drug Design working group is to start planning for a follow-up meeting in 2024. Next time, the meeting will be organised in connection to an advanced PhD-course on drug design.

– Joining these two activities yield many positives. Many of our participating students said that they really enjoyed the opportunity to discuss their work with others, and we want to give people this chance again to meet with different researchers connected to their area of interest.

Raminta Venskutonyte also hopes to include future developments and aspects on drug design into next year's programme. One such example is the use of artificial intelligence, a field that will continue to grow.

– So much is happening, and very fast too. We will include what is most relevant for our Theme and working group. But, of course, the schedule will only come together in the next few months, she concludes.

Legacy statement – Integrative Structural Biology Theme (ISB)

➤ A Grand Finale of the ISB Theme at Kulturen in May

Link to original article, published in the LINXS website May 22nd, 2022:

<https://www.linxs.se/news/2022/6/22/a-grand-finale-of-the-isb-theme-at-kulturen-in-may>

Early May, when the magnolias are in full bloom throughout Lund, the museum of cultural history is a very nice venue for a conference. Even more so for a community of researchers who have not met for a long time and the ISB Theme was to be concluded. The two days were very successful and an inspiring grand finale.

The feedback after the conference has also shown much appreciation. The program was a good mix of topics and speakers and the quality of the numerous key notes as well as the many short talks created a high level of interaction and cross-disciplinary learnings. There were some speakers who were not able to travel but this was solved by presentations online in the hybrid form that we are learning to master in these post-pandemic times.

“Everything worked very well, and the discussions were lively”, says Karin Lindkvist who has been the Theme leader the last years of the three-year Theme period. “Especially the round table discussion was an eyeopener to many participants. Within Integrative Structural Biology you can approach the same biological problems in so many different angles”.

An important outcome of the ISB Theme is the vision to establish an Integrative Structural Biology Centre (ISBC) at Science Village in Brunnsög. Several speakers at the conference came from similar centres in both Europa and the US. There is a strong belief that a centre in our region would be central to both MAX IV and ESS. The close connections to medical research is a unique strength in how the research results can be transferred to clinical practice.

“For me personally, this is a matter that I feel strongly about and drive at the Faculty of Medicin at Lund University”, says Karin Lindkvist. “We will aim for a close relation with Lund University hospital which is a successful, research institution in addition to working closely with the large research infrastructures in Brunnsög. We have had this in mind, but it was good to have this pointed out by international fellows”.

The ISB centre will be a natural continuation from the Theme, and it is also a matter close to the LINXS Director Trevor Forsyth who moved to Lund from a similar centre in Grenoble. A legacy section on the Theme will be published on the LINXS website and available to the community.

“It was a very nice closing conference with a good atmosphere, constructive dialogues and interaction between the senior researchers and the younger generation. There are very large challenges but also huge gains to be met in the field and there are so many kinds of research studies where you can apply Integrative Structural Biology”, concludes Karin Lindkvist.

- **Legacy statement - The ISB Theme has progressed protein science and made it easier for disciplines to meet**

Link to original article, published in the LINXS website Nov 30th, 2021:

<https://www.linxs.se/news/2021/11/29/the-isb-theme-has-progressed-protein-science-and-made-it-easier-for-disciplines-to-meet>

Former Theme leader, Jens Lagerstedt, and current Theme leader, Karin Lindkvist, reflect that protein science have become much broader than what it was before the Integrative Structural Biology Theme started in 2018. The methods available within the field have also become more known to a larger group of researchers.

– One of the greatest strengths of the Theme is how the different working groups have taken on different shape and direction. It has allowed for a more in-depth exploration of integrative structural biology issues since both advanced researchers and newcomers to the field have been able to join, says Jens Lagerstedt, now head of Rare Endocrine Disorders at Global Biopharm at Novo Nordisk.

Different shape and directions of the working groups

For example, the Amyloid working group has focused on exploring the disease perspective, whereas the Time Resolved Structural Biology working group has investigated how one can co-develop and improve beamlines by bringing together physicists and experimentalists. The Membrane Proteins working group, in turn, has worked with supporting researchers to choose suitable integrative methods for their science. The Theme's latest working group, the Lund Integrative Structural Biology Centre initiative (LISBC), aims instead to establish a centre for structural biologists in Lund and to attract international researchers. The Theme has also organised two very successful symposia with invited speakers from all over the world, to showcase the possibilities within the field and initiate collaborations across disciplines and countries. A specific focus for the symposiums has been to highlight the importance of exploring – and using – complementary techniques to better ingrate scientific approaches.

– Someone said to me; everyone is working with integrative structural biology! To us, this is proof that our Theme has made a difference. The fact that the integrative methods are more widely known is a significant achievement, now researchers can go to the structural biology method that best fits their needs, says Karin Lindkvist, core group leader of the ISB Theme, and professor in Medical Structural Biology at Lund University.

Jens and Karin note that a lot has happened in the field overall, which has made it easier for more people to use different methods, for example macromolecular crystallography, Cryo-EM, that although it is not a neutron or X-ray method, has helped open up the field to clinical people, not just experts in structural biology.

Medical and biological questions have come together

Apart from broadening the science and introducing the use of methods to more people, another important milestone for the Theme is that it has brought different questions to meet the right expertise and technology. Medical and biological questions have come together and have benefitted from a transdisciplinary perspective. Examples are new ideas on what can be done in terms of addressing key questions in life sciences, and deeper discussion on what is important to investigate to progress structural biology.

The impact on the broader scientific landscape has also been notable. The Theme has placed LINXS and Lund on the map as a strong research hub for integrative structural biology research. This impact will be even more keenly felt if the LISBC working group manages to establish a special centre for national and international structural biology researchers. Such a centre can progress the science even more, and work towards getting bigger grants and funding, believe Karin and Jens.

– LINXS is absolutely the right place to facilitate new ideas and spark initiatives. And with Trevor Forsyth as new Director, with his experience of building up a similar centre, Partnership

for Structural Biology, at the ILL in France, we have access to great experience in terms of how to go forward, says Karin Lindkvist.

Curiosity and commitment are key

What do Jens and Karin think is key for a Theme to succeed? Curiosity and commitment, they respond! Without a genuine interest, and passionate people, a Theme will simply not work.

Another important factor is to have researchers from other universities and from other countries be part of the core group of a Theme. A regional and international collaboration around activities allow for more networks to be formed, and for new science to develop.

– A challenge for all of the Themes is of course that the activities are mainly performed on a voluntary basis, but one idea for future Themes could be to establish different types of support for Themes, such as mentoring for new Themes, says Jens Lagerstedt.

– Many people who come to LINXS are exploring things they have not done before, and if you learn something new you don't know how long time it will take. This might be a barrier for joining a working group. Having a mentor to bounce ideas off could shorten the learning curve, or at least make the process of setting up a working group smoother, adds Karin Lindkvist.

Support to identify grant opportunities and clarity on Theme activities.

Another way to support Themes could be to encourage them to work on joint publications and help them to identify grant opportunities where they can get further funding to perform more hands-on science. LINXS can thus work like an incubator which seeds larger projects. However, Themes and working groups also have their lifetime, and it is not a given that they should continue indefinitely, reflects Jens Lagerstedt.

Karin Lindkvist also highlights that it could be an option for LINXS to become more inclusive when it comes to methods. Today, the focus is mainly on neutrons and X-rays, but many methods, such as Cryo-EM, are being developed that could be of interest to discuss within LINXS.

Jens and Karin emphasise that it is important to define the economical boundaries of the Themes before they start, as well as looking into having Themes running for different lengths of time if it could benefit a Theme. Another factor is to make sure that new Themes and working groups have a clear idea of what they want to achieve so as to get the most out of their time at LINXS.

– One needs to keep communicating about LINXS to get more people involved. More communication and more outreach to showcase what LINXS can do, and what the Themes have done, is key to get passionate researchers on board, Jens Lagerstedt concludes.

Highlights - Collaboration

➤ **The Lipid Bilayers at ESS Conference (BESS): Expanding the Scope of Biological Membrane Research**

Link to original article, published in the LINXS website Sep 30th, 2022:

<https://www.linxs.se/news/2022/9/29/the-lipid-bilayers-at-ess-conference-expanding-the-scope-of-biological-membrane-research>

With more than 85 people attending the recent Lipid Bilayers at ESS conference, Professor Tommy Nylander concludes that the event was a great success. It was organised as part of a series of conferences gathering researchers globally who work on biological membranes, biophysics, and modelling.

The conference was also the very last event organised by the Dynamics Theme.

He reflects that the event has expanded in scope since it was first organised by ISIS, Rutherford Appleton Laboratory, Oxfordshire, UK, in 2009.

– What started as a neutron focused event has now grown into a broader approach where we highlight both modelling and complementary techniques. I think this is great since it opens up the network, and the research on biological membranes to more people, says Tommy Nylander, professor at Physical Chemistry at Lund University, and LINXS fellow.

Broad programme on science, tools, and methods.

The conference included sessions on biological membranes and functions, membrane structure and self-assembly, membrane dynamics, structural analysis of membranes and lateral and non-planar membrane structures. It also highlighted talks on the role of membranes in health and disease, membrane protein interactions, and application of membranes. Methods and tools were also discussed, such as the need to combine modelling with experiments, how to make full use of the advantage of neutron techniques, by deuteration of lipids, and ways to reduce the background in different sample environments.

In three years, the network will meet again. Tommy Nylander hopes to see an even broader programme at that event. Because more research is absolutely crucial to progress fundamental understanding on how structural biological membranes function.

Research gaps need to be addressed.

Some of the research gaps he would like to see addressed in the coming years, covers areas such as structure/ function relationships, including how to match model systems to real membranes, how to tackle more scarce but crucial lipids, the role of curved membranes and responses to physiological environments, for example enzyme action on biological membrane, and interaction with other components.

More fundamental knowledge will continue to inform the development of a broad range of applications, from the formulation of more effective vaccines to the development of new antibiotics medicines.

– For me personally, these two areas are the most interesting. If we know more about the structure of biological membranes, we can for example develop how we design the capsule

which is used to deliver mRNA vaccine to the body. Many modern vaccine formulations are lipid based, so the opportunities here are endless.

– We also need better understanding of the structure of some bacterial membranes to be able to ascertain why some bacteria tribes develop a resistance to antibiotics. Worldwide, the need for a new chemical compound is really urgent, he concludes.

About the Dynamics Theme.

The Theme "dynamics" addressed time dependent phenomena, such as biological processes, motion of biomolecules and colloids, or transport processes in hard matter, utilizing the accessible time and length scales with neutrons and X-rays, and the coherent properties of MAX IV. Systems and processes studied included equilibrium as well as non-equilibrium phenomena, reversible and irreversible processes, order-disorder transitions, dynamics on different length and time scales, as well as transient states that could for example be studied with pump-probe experiments.

➤ **Gudrun Lotze is Improving the Future Sample Environment at the LoKI Instrument at ESS**

Link to original article, published in the LINXS website Jan 31st , 2023:

<https://www.linxs.se/news/2023/1/31/improving-the-future-sample-environment-at-the-loki-instrument-at-ess>

From 2021 to 2022, LINXS and Lund University hosted guest researcher Gudrun Lotze. She has been working in collaboration with previous LINXS fellow Cedrick Dicko on a joint ESS and Uppsala University project aiming to improve the first future sample environment at the LoKI instrument at ESS. LoKI, which is a Small-Angle Neutron Scattering (SANS) instrument, will be one of the first instruments available to users at the ESS, which is set to open in 2026.

– My main task was to improve the data processing and analysis aspects of a new sample environment available at LoKI. The so-called NUrF sample environment combines Neutron Small-Angle Scattering experiments with simultaneous UV-Vis, Raman, and Fluorescence spectroscopy experiments. The aim is to improve the data quantity and quality of a SANS experiment so that the user will be able to know exactly what happens to the sample at any point in time while the sample is exposed to neutrons, says Gudrun Lotze.

Overcome challenge of huge amounts of data.

Gudrun Lotze explains that there is usually a lot of data generated during neutron experiments. If you do not have data application routines in place to analyse and visualise the measured data immediately, it will be hard for the user during a beamtime to get an understanding of changes within the sample, especially if the sample is exposed for a longer period of time with neutrons. This is because all data points originating from the sample will be averaged during the exposure with neutrons. One way to overcome this, is to apply additional and complementary techniques such as UV-Vis and fluorescence spectroscopy, where the exposure time is significantly shorter than the exposure time with neutrons. This will enable the user to understand what happens to the sample at all points in time, e.g., if the sample undergoes spontaneous changes. Those changes would otherwise not be observable with neutrons alone.

New code will enable observation of the electromagnetic spectrum of a sample.

– I have written software, mainly using scipp, which is a Python library developed directly at the ESS, to process and analyse fluorescence and UV spectroscopy curves that will enable the user to observe large parts of the electromagnetic spectrum of a sample. I have based my code on experimental data measured at other neutron facilities, in this case at the D22 instrument of the ILL neutron facility in Grenoble, France. We aim to pitch this new software to other neutron facilities that also offer the NURF sample environment to their users. The major advantage is that users will be familiar with the sample environment and the dedicated software tools at each facility.

Best practice has guided the work.

Following best practices in software development and expertise in coding are crucial skills in the development of new online analysis tools for instruments, according to Gudrun Lotze. Especially, since there are many challenges related to data extraction and providing, almost in real time, the right information to the user. For example, how to extract the intensity at a certain wavelength provided by the user and relate it to the behaviour of a protein in solution?

– I have really enjoyed working on this project. I like the complexity and diversity of large-scale facilities. You meet many different people: engineers, instrument scientists, external users of highly diverse backgrounds, and software developers. It has been a good experience as instrumentation for sample environment development is so much about teamwork.

The project was led by Cedrick Dicko, Associate Professor at the Division for Pure and Applied Biochemistry, Chemistry Department at Lund University, in collaboration with Professor Adrian Rennie, Uppsala University, instrument scientist Dr. Judith Houston, ESS, and Dr. Gudrun Lotze, previously Uppsala University, now Malmö University.

➤ **LINXS can Play a Role in Disseminating the New Possibilities Afforded by ForMAX**

Link to original article, published in the LINXS website Dec 13th , 2022:

<https://www.linx.se/news/2022/12/12/linxs-can-play-a-role-in-disseminating-the-new-possibilities-afforded-by-formax>

In November, the ForMAX beamline at MAX IV officially opened for user experiments. The beamline is especially designed for advanced studies on wood-based materials, but can also be used for research on food, textiles and within life sciences. Beamline manager Kim Nygård, previous LINXS fellow under the Dynamics Theme, can see many ways in which LINXS can support dissemination of the new possibilities afforded by ForMAX.

– From a technical point of view, ForMAX will provide some unique means for structural characterisation of materials, in particular multiscale, from nm to mm length. It can be used to study processes in situ, and is suited to investigate a range of fibrous materials, says Kim Nygård, researcher at MAX IV Laboratory and beamline manager for ForMAX.

LINXS can help disseminate possibilities afforded by ForMAX.

While he expects a big demand for the new beamline, which just had its first user call, he believes that LINXS can play an important role in disseminating the new possibilities afforded by ForMAX to different user groups.

– At LINXS, many different researchers work in Themes to progress science related to X-rays and neutrons. It is a good setting to highlight how ForMAX can support new science, especially related to food and life sciences. It can also be a place for discussion of how the X-ray experiments at ForMAX can be complemented with simulations and other techniques and tools.

User community existing of both academics and industry users.

Kim Nygård is especially glad that the beamline is an initiative where several market-leading industry companies, mainly from the paper and pulp industry, and academia have joined forces.

– We now have a user community consisting of not just academics, but of industry users too. That really excites me. That means that we can work on different time scales in terms of impact. On the one hand we try to progress basic research questions, where we solve problems within a time frame of 15-20 years. On the other, we have the industrial perspective, where we are aiming to see applicable results in only two to three years.

– It is great that we can now address both needs with ForMAX, and I am very much looking forward to see what comes out of the experiments over time, he concludes.

About ForMAX

ForMAX allows in-situ multiscale structural characterization from nm to mm length scales by combining full-field tomographic imaging, small- and wide-angle X-ray scattering (SWAXS), and scanning SWAXS imaging in a single instrument. The beamline operates at 8-25 keV, with a beam size at the sample of $\approx 1\mu\text{m} - 5\text{ mm}$ depending on mode of operation.

ForMAX is funded by the Knut and Alice Wallenberg Foundation and Swedish industry via Tresearch – a national platform for research on new materials and speciality chemicals from forest raw material. The beamline is accessible for both Tresearch members and general users through the MAX IV user program.