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#### Words from the Director Trevor Forsyth

A (belated) Happy New Year to all of you! At LINXS, we are looking forward to a busy spring term. We have an array of thematic activities, guest seminars, ongoing webinar series, and hosted events planned for the coming months. We are also looking into the details of our short, medium, and long term development plans. Very importantly for LINXS, we have just confirmed the recruitment of a very talented Activities Coordinator – more details in the next issue of the Newsletter after it is all fully formalised.



We are happy to see that the LINXS guest researcher programme is really picking up after the pandemic. In January, we welcomed the first of five guest researchers,<u>Samuele Masoni</u>, a PhD student in Medicinal Chemistry from the Department of Pharmacy at the University of Pisa. He is a junior fellow and has been invited to LINXS as part of the Integrated Pharmacology and Drug Discovery (IPDD) theme; he will stay at LINXS until June.

From April to June, he will be joined by <u>Michael Adams</u> from the University of Luxembourg, who will work with the New Materials theme, and from May to June, by <u>Andreas Stadler</u>, a senior scientist at Jülich Centre for Neutron Science (JCNS) at Forschungszentrum Jülich,

who will also visit in connection with the IPPD theme. LINXS will also welcome <u>Andrew</u> <u>Boothroyd</u> as a guest researcher in May/June. Andrew is a Professor of Physics at the Clarendon Laboratory at Oxford University, and a member of the LINXS SAB. Finally, <u>Prof</u> <u>Carlos Campos</u>, Federal University of Santa Catarina, Brazil, is expected after the summer, from August to October, to work with the New Materials theme. During these visits, a number of seminars and events will be organised to highlight and promote particular areas of science and their engagement with MAX IV and ESS.

The forthcoming LINXS guest seminars are continuing of course. On the 13th February, Nicoló Dell'Unto, Professor in Archaeology, and scientific coordinator for the Lund University Digital Archaeology Laboratory, will give a seminar entitled <u>Recording Visualizing</u> <u>and Interacting: Using Virtual Reality for Interpreting the Past</u>. His lecture will be of wide general interest but perhaps of special interest to those of you working on geoarcheology related science. On the 28th March, Kristina Djinović Carugo, the new Head of the EMBL Grenoble Outstation, will give a more biological seminar on <u>Order from disorder in</u> <u>sarcomeric Z-disks</u>. On 30th March, Adam Hitchcock from McMaster University, in Canada will present on <u>Recent advances in soft X-ray spectro-ptychography</u>. You are most welcome to all these events, and please encourage others to come as well. If possible please use the registration facility so that we can make sure that enough coffee/snacks etc are available – but come anyway even if you have forgotten to do this!

Elsewhere in the Newsletter you will find some reflections on two recent thematic events, the <u>2nd Time Resolved Structural Biology workshop</u>, the final event within the Integrated Structural Biology (ISB) theme, and the <u>Structure Based Drug Design meeting</u>, within the IPDD theme. It is great to see that our events are plugging key gaps, and creating new and important national networks.

In other news, the LINXS SAB has been reviewing the applications to the new <u>national and</u> <u>international Theme Call</u> for which several applications were received. The review process has proceeded to the second stage and the final outcomes will be announced in the end of March. This is likely to result in the expansion of thematic activities and a broadening of the LINXS engagement and remit both nationally and internationally. In addition to this, LINXS has applied to the Swedish Research Council for funding to become a national *Centre of Excellence*. A LINXS Centre of Excellence would resource LINXS Themes driven by PIs from any institute in Sweden - something that strongly complements LINXS' new open call development and our other development plans. We are currently discussing our move to the Science Village at Brunnshög with key potential contractors. LINXS on the Science Village will be placed directly between, and in close proximity to, the MAX IV and ESS facilities. This is all happening at a crucial time during which growth in the area associated with institutes all over the country and beyond is being planned.

A final note on our LINXS calendar: a new calendar has been installed on the website that should help find information about LINXS events and other activities – bear with us while this is populated and automated. Not everything is there just yet!

Take care and stay safe!

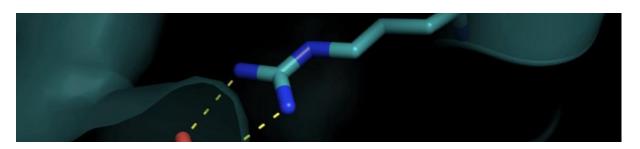


### LINXS Guest Seminar - Recording visualizing and Interacting: Using Virtual Reality for Interpreting the past with Nicolo Dell'Unto

Over the past two decades, visualisation and recording technologies have significantly impacted how scholars perceive and interact with archaeological information. In particular, introducing new visualisation techniques and devices have allowed researchers to experience new ways of simulating the past, creating the conditions for discussing new theoretical frameworks and addressing further research questions.

This talk will discuss the potential, limitations and future developments of 3D visualisation systems as a medium for analysing and discussing archaeological interpretation. **Nicoló Dell'Unto** is Professor in Archaeology and the scientific coordinator for the Lund University Digital Archaeology Laboratory DARKLab.





#### Meeting on Structure based Drug Design provided a good opportunity to build national networks

In mid-November, the Structure-based Drug Design working group, within the theme IPDD, invited researchers to a meeting on structure-based drug design.

– 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, says Raminta Venskutonyte, working group leader, and Assistant researcher at Medical Structural Biology, Lund University.

#### Read an interview with Raminta Venskutonyte about the meeting



### The 2nd Time-Resolved Structural Biology workshop filled important gaps and opens up for future gatherings

Thomas Ursby, researcher, and project manager for the MicroMAX beamline at MAX IV, reflects that the three-day workshop was a great success. Not least being able to meet in person, and having the opportunity to continue discussions during breaks and coffee.

– Many people have mailed to me to say that they really enjoyed the workshop, and that they gained a lot from attending. Getting this this type of feedback is really nice, and an indication that our scientific programming is of value to the research community, says Thomas Ursby.

Read an interview with Thomas Ursby about the meeting

### LINXS welcomes junior guest researcher Samuele Masoni

Samuele Masoni is a PhD student in Medicinal Chemistry, Department of Pharmacy, University of Pisa (Italy).

He is invited as part of the work within the IPDD theme as junior guest researcher and LINXS fellow. He will stay at LINXS from January unto June. His research is focused on the synthesis of novel small molecules interfering with cell metabolism, particularly glucose and lipid metabolism, applied in relevant pathologies, such as neurodegenerative and cancer diseases.

Read an interview with Samuele Masoni





### Improving the sample environment at the LoKI instrument

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.

Read an interview with Gudrun Lotze about the project and her work

## Calendar

Our upcoming scientific activities within our Themes and Working Groups, and related events.



Antibodies in Solution: a LINXS – NIST Webinar Series

- Structural Bioinformatics, with Sergej Grudinin, CNRS, France

<u>Register</u>



CoWork series:

- HPC+AI@Edge Enabled X-ray Science at The Advanced Photon Source, with Mathew J. Cherukara, Argonne National Laboratory

Register



LINXS guest seminar:

- Recording visualizing and Interacting: Using Virtual Reality for Iterpreting the past with Nicolo Dell'Unto

<u>Register</u>

**15** Feb

LINXS related event

- CIPA: Spectroscopic Data Processing and Analysis

<u>Register</u>

# **23** Feb

#### CoWork series

- Aline Ribeiro Passos, The Brazilian Synchrotron Light Laboratory (LNLS)

Save the date



Antibodies in Solution: a LINXS – NIST Webinar Series

- NMR, with John Marino, Nist, USA

Save the date

**7-9** Mar

Northern Lights on Food

- Image Analysis Hackathon - with the Structure of Food During Processing working group

<u>Register</u>

<b>13</b> Mar	LINXS Young researchers' symposium - Life Sciences Save the date
15- 17	LINXS partner event - MATRAC School <u>More information and register</u>

<b>20-</b> <b>23</b> Mar	LINXS related event - European Conference on Neutron Scattering 2023 More information and register
<b>20-</b> <b>24</b> Mar	New Materials - LINXS XAS-School 2023, Charge Transfer Materials working group Register
<b>28</b> Mar	LINXS guest seminar - Order from disorder in sarcomeric Z-disks with Kristina Djinović Carugo, EMBL <u>Register</u>
<b>30</b> April	LINXS guest seminar and WEBINAR: CoWork series - Recent advances in soft X-ray spectro- ptychography with Adam Hitchcock <u>Register</u>
<b>5</b> April	Antibodies in Solution: a LINXS – NIST Webinar Series - Domain Motions, with Ralf Biehl, Jülich Centre for Neutron Science (JCNS), Germany

	Save the date
<b>12</b> April	LINXS outreach event - ATLAS Career Fair 2023 More information
<b>19</b> April	Northern Lights on Food theme - Workshop with the Food Interaction on Surfaces working group Save the date
<b>20</b> April	LINXS outreach event - HALRIC Hanseatic Life Science Research Infrastructure Consortium, kick off meeting More information
<b>2-3</b> May	New Materials - Catalysis workshop <u>Save the date</u>
<b>3</b> May	Antibodies in Solution: a LINXS - NIST Webinar Series - All Atom MD with Christina Bergonzo, Nist, USA

#### Save the date

<b>4</b> May	LINXS Science Day <u>Register</u>
<b>24</b> May	Integrative Pharmacology and Drug Discovery - Theme meeting <u>Save the date</u>
<b>26</b> May	Integrative Pharmacology and Drug Discovery - Workshop on Biomedical Imaging <u>Save the date</u>
<b>7</b> June	Antibodies in Solution: a LINXS - NIST Webinar Series - Protein Interactions with Mikael Lund, Lund University, Sweden Save the date
<b>7-9</b> June	Northern Lights on Food - Northern Lights on Food - Conference IV <u>Save the date</u>



LINXS outreach event

- BSR14 - 14th International Conference on Biology

and Synchrotron Radiation

Save the date

MORE LINXS ACTIVITIES