Protein Science Day 2019 – Measuring interactions: from molecules to cells

15th October 2019

Lund University, Sweden

Hosted by Molecular Recognition in Life (MoReLife), HALOS, ESS, and MAX IV

Co-sponsored by Dynamic Biosensors, Xtal, NanoTemper, and GE Healthcare Life Sciences

Location: Belfragesalen, BMC

09.00 Welcome

09.10 “The Correlative Image Processing and Analysis platform”, Jonas Ahlstedt

09.20 “Lund Institute of Advanced Neutron and X-ray Science (LINXS)”, Jens Lagerstedt

09.30 “Hanseatic League of Sciences - HALOS”, Kajsa Paulson

09.40 "In situ Dynamic Light Scattering: A time and sample efficient method to qualify samples for Crystallization, SAXS, NMR, SPR and Cryo-EM", Xtal-concept (Sponsor), Arne Meyer

10.00 “The switchSENSE® biosensor platform for the analysis of molecular interactions”, Dynamic Biosensors (Sponsor), Thomas Welte

10.20-11.05 Coffee and tea +

Instruments demo (room 1 and 2) at D15 or

HALOS speed-dating (meet representatives from HALOS e.g., MAX IV, ESS, the Lund University HALOS reference group and others, present your science case and get suggestions on techniques and/or who to contact for applying synchrotron, neutron and FEL methods. Sign up for this part and we will match you with one or more HALOS representatives for a 5-15 minutes discussion), Dora Jacobsson or Bengt Borgström at D15 or conference room at D14 or C14.

11.05 “The nitty-gritty of molecular interactions”, Mikael Akke

11.25 “New synchrotron-based tools to study time-resolved protein-protein and protein-ligand interactions”, Arwen Pearson, Hamburg

11.45 “Challenges and opportunities in biologics”, Marie Wahlgren

12.05 “Let’s hear from the young researchers” (postdocs/Ph.D. students give short presentations)

“Modelling the core of lipid nanoparticles encapsulating messenger RNA”, Giulio Tesei

“FragMAX: Fragment Screening platform at BioMAX”, Gustavo Lima, MAX IV

12.25 “Live-cell interfaces with nanomaterials”, Christelle Prinz

12.45-13.30 Joint lunch + *(Instrument try)*

13.30 “Structural mass spectrometry”, Sven Kjellström

13.50 “Resolving protein-nucleic acid interactions during viral capsid assembly using small-angle scattering and cryoEM”, Ryan Oliver

14.10 “Multi-molecular organisation and architecture: How cells encode information as they move”, Vinay Swaminathan

14.30 “Let’s hear from the young researchers” (postdocs/Ph.D. students give short presentations)

“How ligand densities and ligand mixtures can affect protein affinities within a cell contact”, Victoria Junghans

“*In vivo* engineering of human hematopoietic niches as advanced screening platform”, Ani Grygorian

“SoftiMAX: A new imaging beamline at MAX IV”, Jörg Schwenke, MAX IV

15.00-15.30 Coffee and tea + *(Instrument try)*

15.30 " Methods for structural characterization in 3D within QIM”, Anders Bjorholm Dahl, DTU

15.50 “A bacterial virulence factor that hijacks plasma proteins to modulate host cell function”, Oonagh Shannon

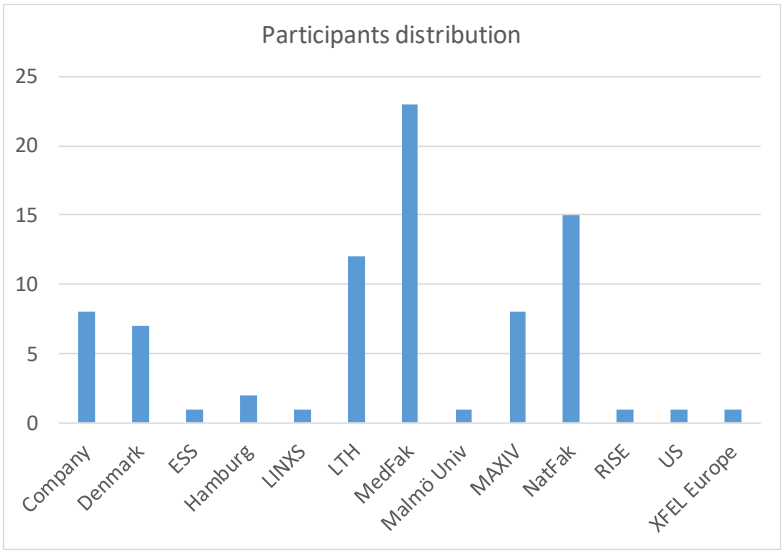
16.20 Discussion in smaller groups

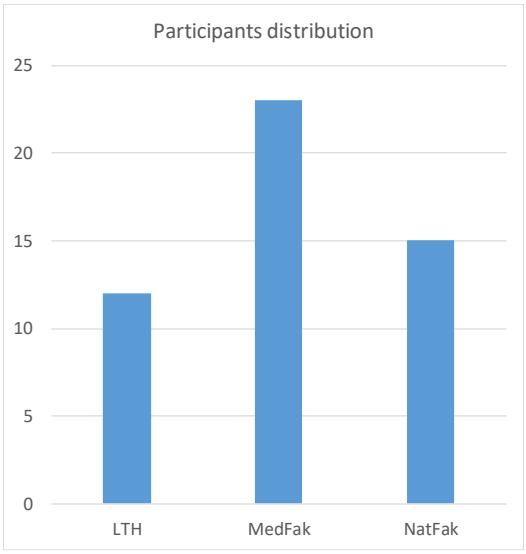
16.40 Sum up and concluding remarks

17.00 Tapas, drinks and mingle

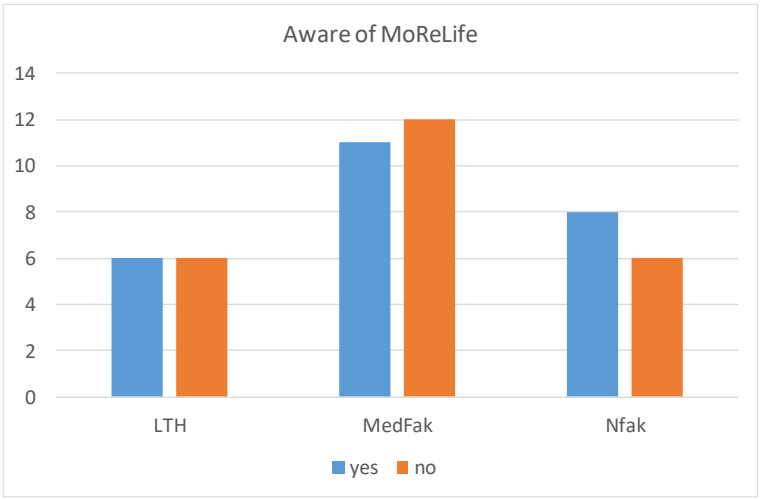
Survey questions and answers

1. Participants (in numbers)

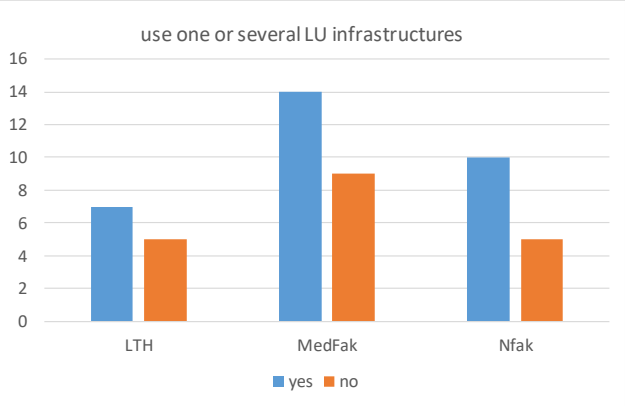


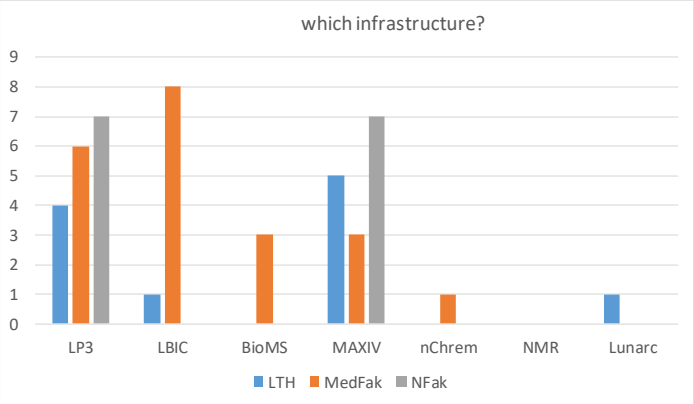


2. Were you earlier aware of MoReLife? (in numbers)

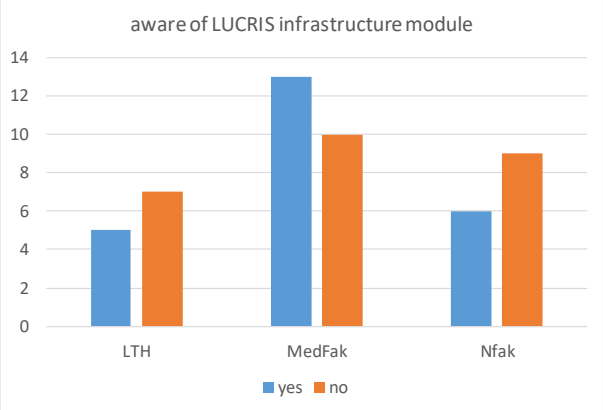


6. Do you use any of LU's infrastructures (e.g., LBIC, LP3, MAX IV, other)?

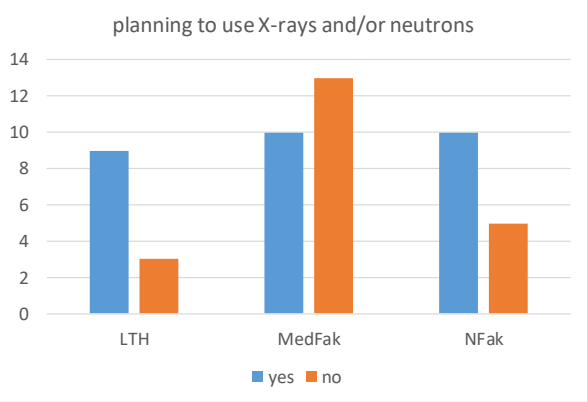


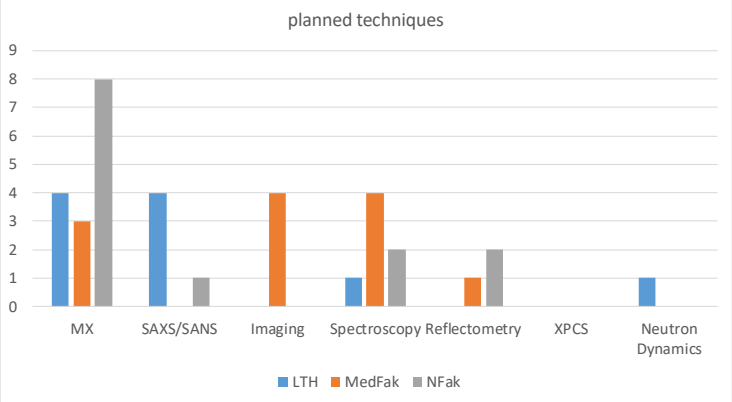


7. Are you aware of the Infrastructure search module in the LU research portal?



8. Have you or do you plan to in the near future use synchrotron light or neutrons? If yes: What type (e.g., crystallography, imaging, spectroscopy or something else)? If yes: What type (e.g., crystallography, imaging, spectroscopy or something else)?





10. Which Infrastructure(s) are missing at LU?

"computation, Crystallography (not crystallization, but the staff that can provide systematic help for structure solving, etc)"

“Drug screening facility.”

“information about available infrastructures”

“single-particle cryo-EM microscope”

“an in situ DLS plate reader for very small volumes”

"Dianthus NT.23 for affinity screening in well plates Tycho NT.6 for QC "

“Bio-medical imaging beam-line.”

“BIOSAXS”

“We need to further develop image processing and analysis.”

“We need resources for single-particle cryoEM sample preparation, screening, and analysis (and eventually also a high-end instrument for analysis).”

“We need a BioSAXS”

11. The suggestion of topics to discuss

Edited Discussion Topics

1. General

- Infrastructure co-use?
- How to find experts?
- What to do when we have too much data?
- What developments/infrastructures are missing at LU for structural biology?
- How to secure resources for our needs?
- How can we best make use of existing resources - networks, user forums, discussion groups?

Industry and European projects

- Interactions industry / academia / large scale infrastructures?
- What to do after HALOS, are there funding options for long-term collaborations?

2. MAX IV and ESS

- What is the potential new research path that LU, together with MAX IV and ESS, can follow?
- What are LU long term plans regarding science around MAX IV and ESS?
- MAX IV and; ESS overview talks [in a nutshell] (current status, the outlook for the next 1-2 years): maximum 30 minutes each, just a short appetizer

3. Techniques

- How to measure electron transfer
- Time-resolved spectroscopy techniques

- The relevance of Dianthus NT.23 as orthogonal screening method to SPR - that works well for transmembrane proteins and small mass changes in case of small molecule- or fragment-binders.

- the relevance of the label-free nanoDSF for protein characterization/QC (unfolding, aggregation of different batches/conditions) before expensive analyses at MAXIV or even CryoEM - to increase efficiency and high-quality data.

- Sample quality?

4. Imaging

- How to image bacterial surface proteins (and interaction between them) using whole native (environmental) strains. Potential new methods, in particular, in the region.

- Tomographic imaging at MAX IV and its relation to analysis resources.

Summary of PSD 2019 discussion

The PSD discussion session included selected points from topics suggested by the almost 100 participants.

Information dissemination

We have a big challenge at the faculty/university/organization level to improve the spread of information. There is a problem both to send out and receive information, and this is shared between the organisations participating in the discussion session of the PSD 2019 (including Lund University, DESY, European XFEL, MAX IV, ESS, industry). It is a challenge, and a paradox that people lack information and very much would like to be informed but at the same time feel they are drowning in information from emails, newsletters, social media.

What to do?

Giving many persons the same information at the same time point will increase the chances that discussions and further dissemination take place by people talking to each other. At Lund University, there is no synchronization between, e.g., the faculty news-letters, they are published at different time points.

Never only refer to a web page or pdfs. There must always be a direct message in emails and newsletters. Researchers might not click on links and read documents – not because of a lack of interest, but they do not have the time.

Custom tailor emailing (tag with key-words to allow people to search for emails). Try to avoid filters since “you might miss out on things that you are not aware you are interested in until you see the email/article”.

Create virtual searchable platforms for questions and discussions.

Make study visits to universities where communication works.

Understand the value of personal contacts: Social interaction is essential. Create venues and events where people meet and get to know each other, e.g., Protein Science Day, pub nights etc. The best way to spread or get information is by talking to someone. This assures that the message is received and also gives an appreciated quality stamp in an era where information includes generous amounts of superlatives without necessarily a solid base or anchoring. Finding experts and collaborators is usually done by personal contacts, not by the net. Advertisement/information on, e.g., websites is not the same as providing information that can be used for judgment of a need (this requires personal contact). We need testimonials and personal recommendations to trust information. Do not underestimate the value of resources for direct contact, discussions in person, for advice on who else to contact for further information regarding expertise, techniques, infrastructures, funding, collaboration opportunities, etc. Communication in real life, by researchers themselves as well as coordinators, “ambassadors,” management, leadership, etc is needed more than ever despite the past decades' advances in information technology.

What to do - LU specific suggestions

Reduce the number of newsletters and emails. Have one joint newsletter for researchers, an LU newsletter/magazine (LUM is for administrative personnel, and not directed to researchers).

Make the LU page searchable. It is complicated to search for information at LU. Even if you know what you are looking for, there is a significant risk you will not find it (e.g., information on a specific seminar, a call for financing, routines for procedures at LU).

Create a joint page for infrastructures. The LUCRIS database is good, but we also need a dynamic LU page or similar information where information is displayed. It is worth noting that only X of the Y number of PSD participants from LU were aware of the LUCRIS infrastructure module.

Resources needed

In connection to different types of infrastructure for wet-lab work, there needs to be easily accessible resources for post-wet lab work — resources for data handling and analysis including resources for writing code. There is a general problem that help is required for the analysis (ideally more resources where non-experts can use black box software to get out information). This is already well developed for some areas, e.g. chemical crystallography, and needs to be further pursued for other types of analysis, including tomographic image analysis. The user communities will not, and should not be required to have the ability to do the analysis themselves. Excellent researchers are not necessarily suitable analysers. We need platforms to assist with analysis and handling of data from large scale facilities and others. This is an absolute necessity to make the large-scale infrastructures the resources they could and should be for the life science community.

Imaging with SR. Discussion included how to match samples to the instruments and methods, where does the contrast comes from, the advantage of having reference material, and the need and challenges of quantification. It was concluded that many would benefit from talking directly with beamline scientists. Beamline scientists are important as experts and also as to facilitate contacts with other facilities.

Industry-academia-large scale facility

We would all benefit from, to a higher extent involve companies when developing new techniques. We should also have more dialogue regarding solutions for new instruments, e.g., the possibility for companies to place instruments at infrastructures and universities. The researchers need to define what the baseline instrument park consists of, and then we should discuss how we could organize resources, etc.

Additional important questions to address are: What are the academic expectations on a large scale facility complementary infrastructure? What should large scale facilities offer to users? Where does the ownership start and end? How to organize access to complementary labs in academia? At European XFEL the user community funded and organized supporting labs.

Several big companies have made a significant investment in sponsoring complimentary facilities and testbeds. Industry recommends "Decide on the partners you want (big players) - and go for it."

The life science community urgently needs its specific voice regarding matters related to the large scale facilities, and with HALOS the life science sector can work together to accomplish our goals, including taking advantage of the large scale facilities. HALOS should be used as a venue to increase interaction between life science industry-academia-large scale facilities and other key stakeholders such as funding agencies and national politicians. Through dialogue, joint activities, communication, and visibility we will develop the Hamburg-ÖKS area to a globally unique life science community for research and innovation. HALOS is a unique tool for the life science community since it includes both regional development actors as well as industry, researchers and large-scale facilities in the same project. HALOS should always be open for joint efforts and collaborations with other initiatives such as LINXS, LINX and also initiatives and projects outside but in proximity to the core HALOS geographical area.

Students need to be connected to the large-scale facilities

We need to create further and develop models for students to join the activities happening directly at the large scale facilities. Mobility programs for students exist, and this is a valuable tool that should be used and further developed. Mobility programs would also be positive for other categories such as beamline personnel. There is a problem of connecting students directly to the facilities and the beamlines. Ideally at least one Ph.D. student should be connected per beamline. The facilities have the option to both host students and involve students affiliated at other organisations.