Statistics of the Protein Science Day 2018

The distribution of the 98 registered for Protein Science Day 2018: **35% FoM, 21% FoS, 12% LTH,** 32 % others (others including MAX IV, ESS etc). For comparison the 67 participants at Protein Science Day 2017 had the following affiliations: **35% FoM, 23% FoS, 12% LTH,** 30% others and of the participants at Protein Science day 2016 had the following affiliations: **17% FoM, 39% FoS, 17% LTH**, 27% others.

The participants of the PSD were asked to write down what infrastructures they would like to have access to at Lund University but that they were missing today:

- **Electron microscopy**
  - Intermediate Cryo-EM to screen before accessing advanced instruments
  - High resolution Cryo-EM available at LU (Stockholm and Umeå have one Talos Artica each)

- **Image processing and analysis (and imaging)**
  - Cloud computing and storage
  - High-content imaging, bio-image analysis
  - Resources, personnel and software (for image processing and analysis)
  - MedMAX (Medical imaging beamline at MAXIV)

- **Bioinformatics**
  - Better visibility for bioinformatics
  - Bioinformatics resources for protein modelling, analysis and simulations

- **Proteins in solution**
  - nanoDSF and MST
  - BioSAXS (at lab, not SR)
  - SR-CD beam line at MAX IV (synchrotron radiation circular dichroism)

- **Mass spectrometry**
  - Ease of access to users and support
  - A bigger and more easily accessible MS unit

- **General**
  - - Increase of staff at existing infrastructures to meet the users need

To follow up on the above list the PSD included an afternoon discussion session.

The discussion was conducted linearly by following the different points in the topics above.

Electron microscopy

To the question of "should Lund have a dedicated cryo-EM for life science?"

- There are EM at LU but may be coordination and visibility is not sufficient. An identified challenge for the existing EM is that they are multi-purpose (from nanomaterials to life science).
- Another identified challenge for existing EM at LU is that they are not automated, thus precluding high throughput. In addition, the detectors used are not well suited for life science.
- A point was made that SciLifeLab recommends that all major universities should have dedicated cryo-EM for screening prior to accessing high-resolution instruments in SciLifeLab.
- Some questions were raised regarding price of a screening cryo-EM and most importantly staffing of such instrument.

- A possibility discussed was hiring a dedicated person for cryo-EM for life science using LU current instrumentation.

Image data storage, processing and analysis

- Related to cryo-EM
  - need for personnel to support users
  - data storage and transport
  - joint backup server for cryo-EM, imaging, bioinformatics
- Generally, it was felt that facilities producing the data should address the issues of data storage and transport. The example of MAX IV and LUNARC on going collaboration was given.
- There is a need to have a dedicated person/effort to drive data storage and transport for LU scientists.

Bioinformatics

- Karin Engström is in the process of defining the bioinformatics community at LU and needs.

Proteins in solution

- The discussion of visibility for the “smaller” instruments was raised. For example nanoDSF and MST are valuable instruments, they are present at LU but not easily found. The new LUCRIS module for infrastructure will solve this problem but the small instruments need to be registered.
- There is a need for a dedicated BioSAXS, the discussion will be taken forward to MAX IV. In the audience, there was a clear will to have a dedicated BioSAXS at LU.
- The possilbility of SRCD at MAXIV on the small ring will be taken forward to MAX IV.

Mass spectrometry

- One support staff each at the faculty of Medicine and Region Skåne financed at 50% is a good start but not sufficient to cover the needs.
- How should MS at LU be coordinated to increase visibility and facilitate accessibility to the correct instrument. Charlotte Welinder already engages with users but there is a need for a coordinator to harmonize the MS activities.
- Question: Should MS at LU be visible differently at the national level? For example with regards to BioMS in Göteborg should find a relevant MS be managed nationally.

General

- Generally, all agreed that the lack of support staff is slowing down the exploitation of the infrastructures resources at LU.
- Mapping of infrastructures at LU, there is a need and it should be discussed how visualisation should look like: by topics, by techniques, etc.

Protein Science Day 2018 – Proteins: from modelling to manufacturing

16th October 2018

Lund University, Sweden

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

Co-sponsored by Malvern and NanoTemper

Location: Belfragesalen, BMC

9.15 Welcome

9.30 "Coordination of bioinformatics at LU", Karin Engström, LU

9.40 "Mass spectrometry at Medical Faculty, LU", Charlotte Wellinder, LU

09.50 "NanoDSF for protein stability and interactions", Rene Wink, NanoTemper

10.10 "Protein characterization using the New Malvern Panalytical Zetasizer Pro and Ultra", Patrick King, Malvern

10.30-11.00 Coffee and tea + *Instruments demo (DLS and Microscale Thermophoresis)*

11.00 "DEMAX: the deuteration and crystallization user support lab of the ESS", Zoe Fischer, ESS

11.20 "Proving ourselves wrong: unusual protonation states and hydrogen bonding in enzymes seen by neutron crystallography", Andrey Kovalevsky, Oak Ridge National Lab

11.40 "Structural mass spectrometry and cryoEM of host-pathogen protein complexes", Lotta Happonen, LU

12.00 "Let's hear from the young researchers" (postdocs/PhD students give short presentations)

To polymerize or to not polymerize- that is the question for intrinsically disordered wheat proteins", Joel Markgren, SLU Alnarp

Serial crystallography at BioMAX beamline", Anastasiia Shilova, MAX IV

12.20 "Modelling of Intrinsically Disordered Proteins: Comparison with SAXS", Marie Skepö, LU

12.40-13.20 Joint lunch + *(DLS and Microscale Thermophoresis)*

13.20 "Possibilities and Challenges in Protein Production", Claes von Wachenfeldt, LU

13.40 "Protein Science at AstraZeneca – cool science in a changing world", Lovisa Holmberg-Schiavone, Astra Zeneca Mölndal

14.20 "Hemoglobin from bench to blood bank", Leif Bülow, LU

14.40 "Let's hear from the young researchers" (postdocs/PhD students give short presentations)

"FragMAX – The BioMAX fragment screening platform for drug discovery", Gustavo Lima, MAX IV

"Protein Perdeuteration in Escherichia coli for Neutron Protein Crystallography", Vinardas Kelpšas, LU

15.00-15.30 Coffee and tea + *(DLS and Microscale Thermophoresis)*

15.30 "Deep mutational scanning as a tool for optimization of protein stability, binding and expression", Ingemar André, LU

15.50 "Engineered botulinum neurotoxin B with improved efficacy for targeting human receptors has improved clinical potential" - Pål Stenmark, LU

16.20 Discussion in smaller groups

16.40 Sum up and concluding remarks

17.00 Tapas, drinks and mingle