Integrative Structural Biology at SciLifeLab Lund

LOKI Early Science Workshop

Wojtek Potrzebowski

Data Science Coordinator

Research Infrastructures in Sweden

MAX IV

ESS EUROPEAN SPALLATION SOURCE

SciLifeLab

What is SciLifeLab?

National hub enabling life science research that would otherwise not be possible.

- Activities at all major Swedish universities.
- Organised in 10 technology platforms and 40 research units distributed nationally.
- Study all molecular aspects of life, from the atomic scale up to entire ecosystems.
- Applicable across a large spectrum of disciplines and research fields in life science

What do we offer?

- Advanced technologies
- Unique instruments
- Expert know-how

Who can access it?

- Academia
- Industry
- Healthcare
- Other governmental agencies
- International users

The Dimensions of SciLifeLab

Research environment

- ~190 affiliated research groups
- 400+ SciLifeLab Group Leaders
- Broad range of science fields

Infrastructure

- 10 technology platforms
- 40 research units
- 1800+ users
- 4300 projects/year
- ~600 technology experts

Data-Driven Life Science

- Accelerating paradigm shift
- 4 strategic research areas
- Recruiting global talent
- Academic and industry PhD and postdoc programmes
- Collaboration, innovation, interdisciplinary science

SciLifeLab Sites

Gothenburg

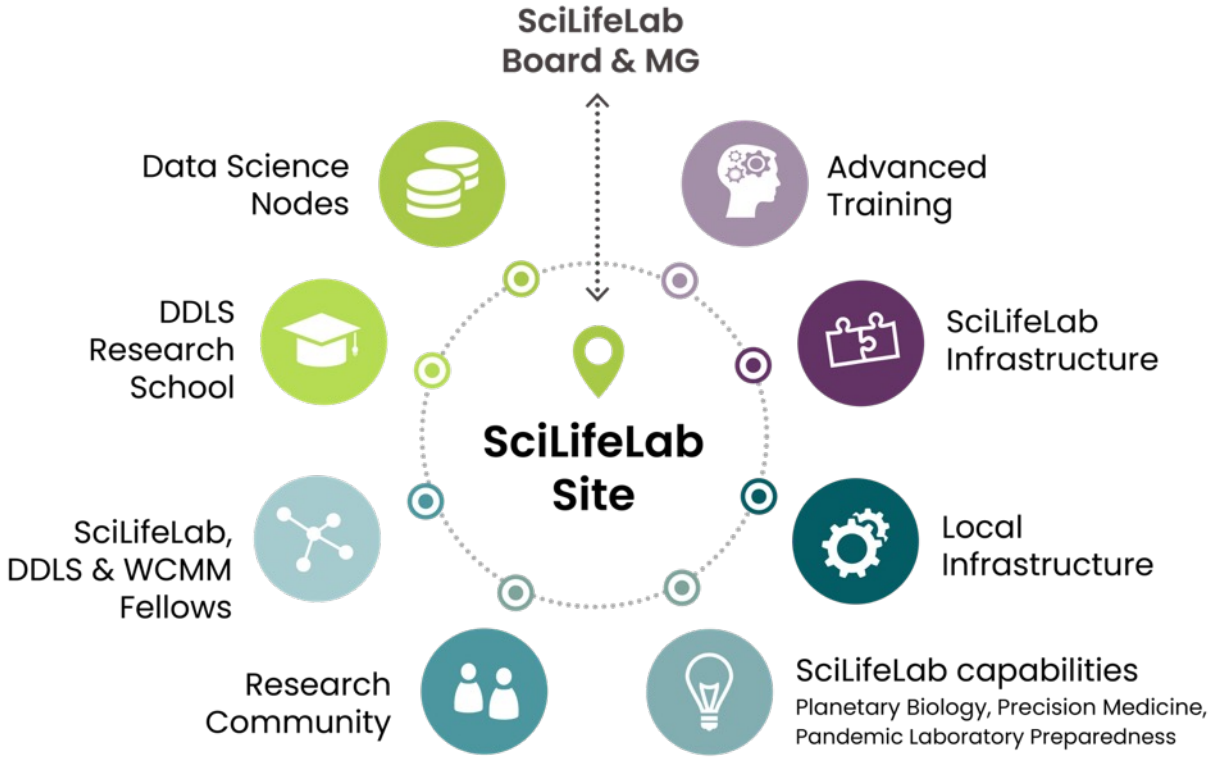
Linköping

Lund

Stockholm

Umeå

Uppsala



SciLifeLab Lund Units

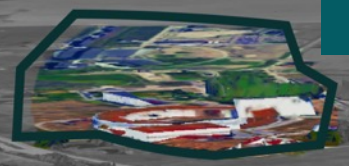
- Clinical Genomics Lund
- Biological Mass Spectrometry
- Chemical Biology Consortium Sweden
- Cryo-Electron Microscopy
- Display and Selection Technologies
- Lund Bioimaging Centre
- Lund Protein Production Platform
- Structural Proteomics
- National Bioinformatics Infrastructure Sweden

Candidates:

- Cell and Gene Therapy Core
- FragMAX
- LU-Fold

Almost all units have activities in Structural Biology

SciLifeLab Lund



European Spallation Source

MAX IV

LINXS

Medicon Village

Faculty of Engineering

SciLifeLab Lund

Faculty of Science

Faculty of Medicine

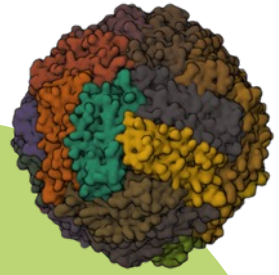
Skåne University Hospital

- Strong **translational** profile with well-established collaborations with Region Skåne
- Unique environment for:
  - **Structural biology** research: MAX IV, ESS, LINXS, LU-fold, Structural Proteomics, Cryo EM, LBIC)
  - **Single-cell** applications

Structural Biology at SciLifeLab Lund

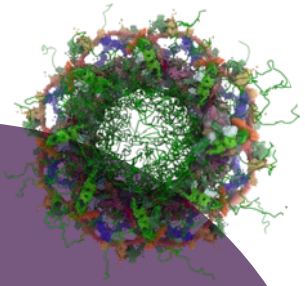
IT Infrastructure

- SciLifeLab cross-platform data harmonization
- Integrative Structural Biology Portal
- Improved user experience
- Building community



Model systems

- Improve already collected data
- Showcase cross-platform capability
- Use data for method development and training

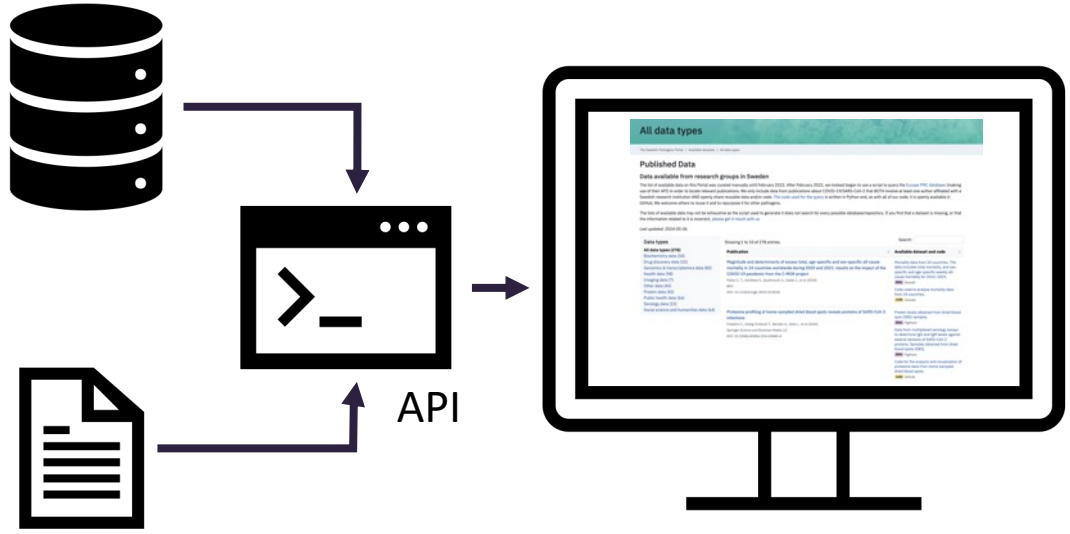


Cutting edge science

- New systems to be identified by the community
- Streamlined workflows
- Exploiting full cross-facility potential

Portal for Integrative Structural Biology

- Data from at least two techniques
- Compatible with PDB-dev
- Coupled with SciLifeLab IT services
- Integrated with MAXIV and ESS
- Can include simulated structures (LU-Fold) and data from FragMax
- Basis for recommendation system and multi-modal analysis



Internal and external
Annotations (PDB-dev, MAXIV and ESS)

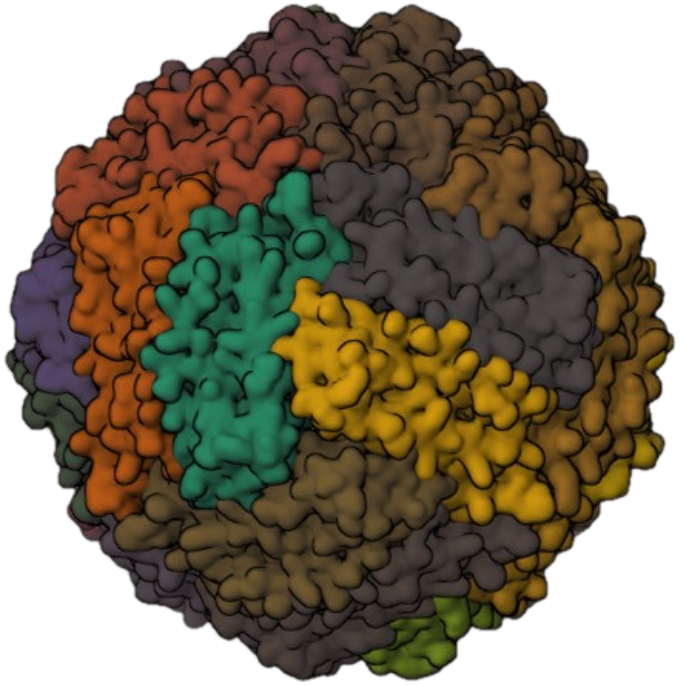
Pathogens Portal for the inspiration

https://www.pathogens.se

Model systems

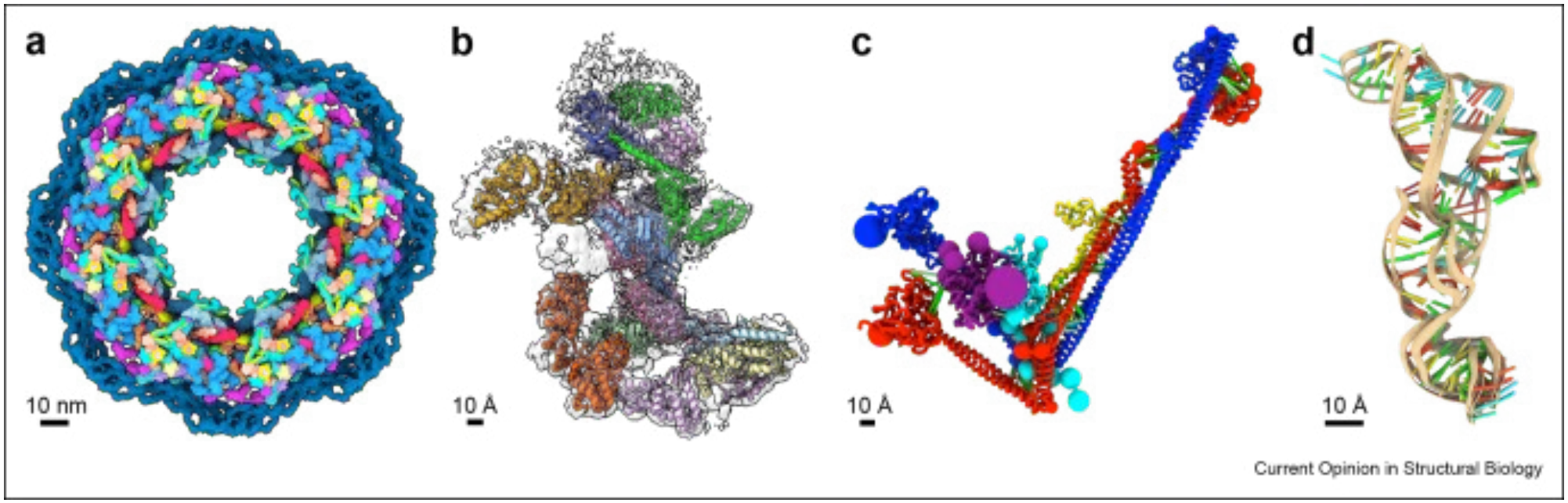
- E.g. ferritin has been studied with multiple techniques but data is scarce
- Potential to “improve” already existing data sets
- New measurements to showcase cross-facility approach
- Basis for method development
- Simple data mining can already identify candidates for SANS

Method	Data available	Publication
X-ray cryst.	🙂	🙂
NSE	☹	🙂
CryoEM	🙂	🙂
MS	☹	🙂
NMR	☹	🙂
SAXS	☹	🙂
SANS	☹	🙂



New systems

- To be defined by the community and SciLifeLab Group Leaders
- Data and metadata collected using SciLifeLab infrastructure
- High-risk experiments supported by developed computational methods



What are the benefits?

SciLifeLab

Well-curated data sets
Cutting edge science
Access to cross-platform and cross-facility experiments
Long-term: closer collaboration with healthcare

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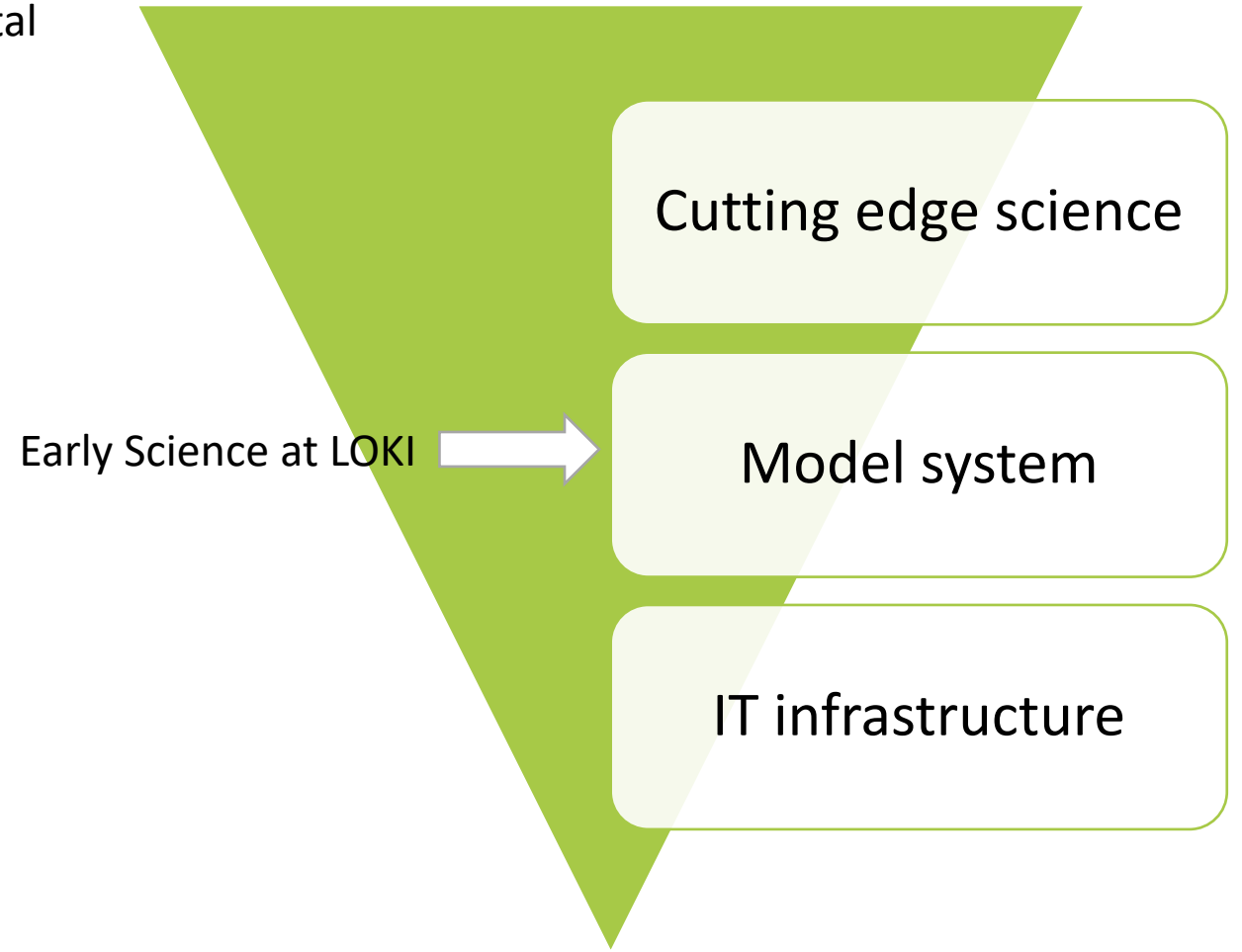
SANS can be used to showcase the approach
Well-characterized biological systems for instrument debugging (including SEC-SANS)
Increased visibility through the recommendation system

How to get involved?

- Join the working group to define the scope of ISB portal
- Provide data for model systems
- Engage in computational method development
- Help with defining new systems



SciLifeLab Lund

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