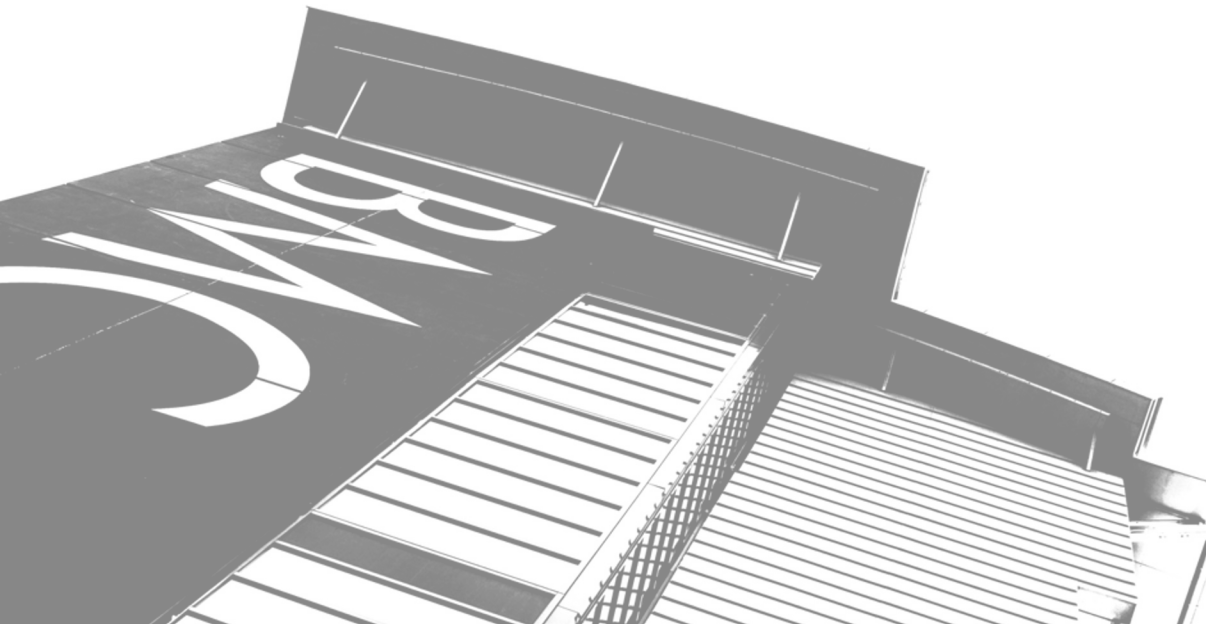


# Integrative Structural Biology at SciLifeLab Lund

LOKI Early Science Workshop

Wojtek Potrzebowski

Data Science Coordinator



# Research Infrastructures in Sweden





# 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

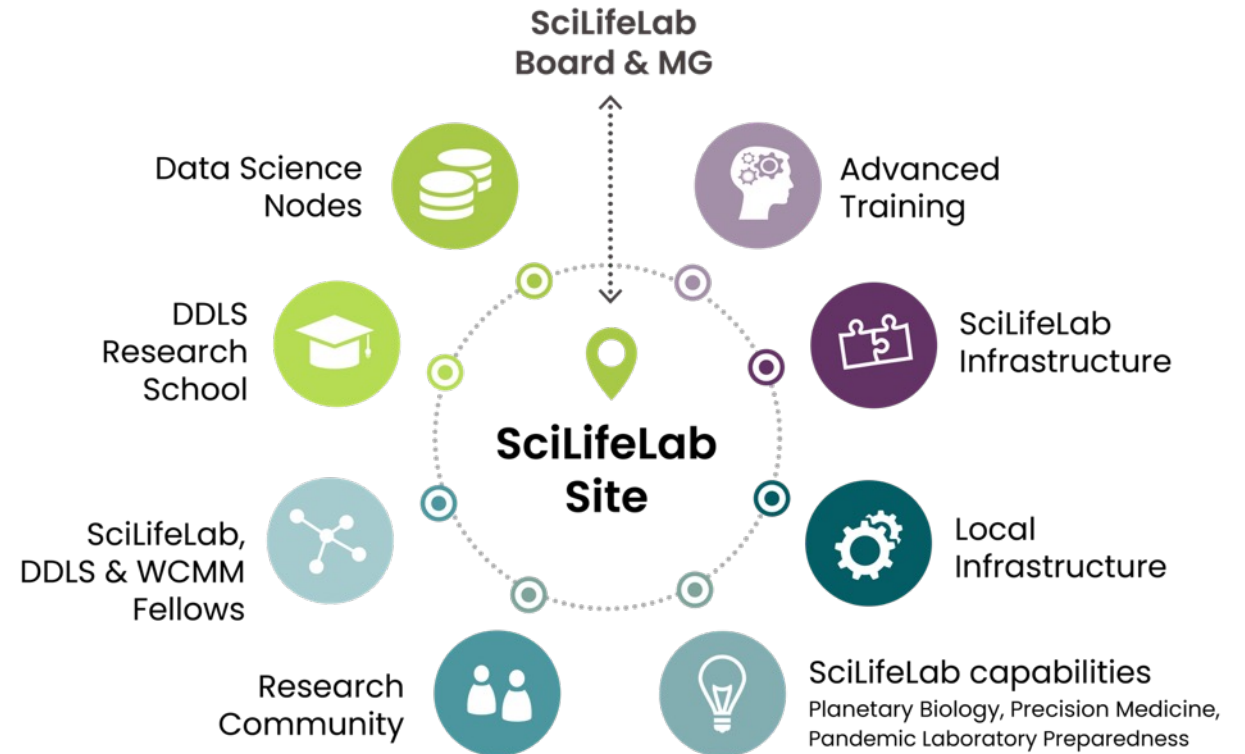
Linköping

**Lund**

Stockholm

Umeå

Uppsala



# SciLifeLab Lund Units



Clinical Genomics Lund



Lund Bioimaging Centre



Biological Mass Spectrometry



Lund Protein Production Platform



Chemical Biology Consortium Sweden



Structural Proteomics



Cryo-Electron Microscopy



National Bioinformatics Infrastructure Sweden



Display and Selection Technologies

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

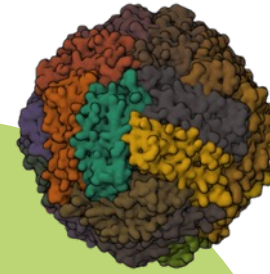


# Structural Biology at SciLifeLab Lund



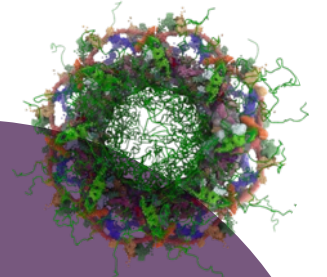
## IT Infrastructure

- 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

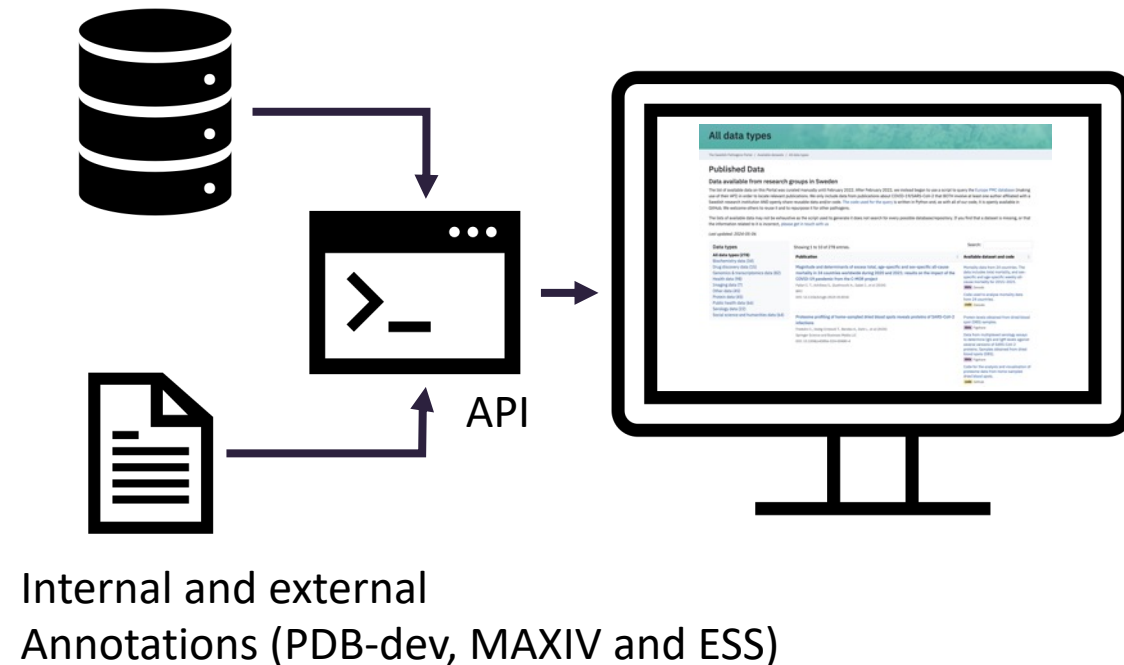
- New systems to be identified by the community
- Streamlined workflows
- Exploiting full cross-facility potential



# 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



# Pathogens Portal for the inspiration



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[Data Dashboards](#) [Research Data Management](#) [Editorials](#)  
[Research & Funding](#) [Sample Collection Database](#) [Events & Training](#)

## All data types

The Swedish Pathogens Portal / Available datasets / All data types

## Published Data

### Data available from research groups in Sweden

The list of available data on this Portal was curated manually until February 2022. After February 2022, we instead began to use a script to query the [Europe PMC database](#) (making use of their API) in order to locate relevant publications. We only include data from publications about COVID-19/SARS-CoV-2 that BOTH involve at least one author affiliated with a Swedish research institution AND openly share reusable data and/or code. [The code used for the query](#) is written in Python and, as with all of our code, it is openly available in GitHub. We welcome others to reuse it and to repurpose it for other pathogens.

The lists of available data may not be exhaustive as the script used to generate it does not search for every possible database/repository. If you find that a dataset is missing, or that the information related to it is incorrect, [please get in touch with us](#)

Last updated: 2024-05-06

### Data types

#### All data types (278)

- Biochemistry data (34)
- Drug discovery data (15)
- Genomics & transcriptomics data (82)
- Health data (98)
- Imaging data (7)
- Other data (45)
- Protein data (45)
- Public health data (66)
- Serology data (22)
- Social science and humanities data (64)

Showing 1 to 10 of 278 entries.

Search:

Publication	Available dataset and code
<b>Magnitude and determinants of excess total, age-specific and sex-specific all-cause mortality in 24 countries worldwide during 2020 and 2021: results on the impact of the COVID-19 pandemic from the C-MOR project</b> Pallari C. T., Achilleos S., Quattrocchi A., Gabel J., et al (2024) BMJ DOI: 10.1136/bmjgh-2023-013018	Mortality data from 24 countries. The data includes total mortality, and sex-specific and age-specific weekly all-cause mortality for 2015–2021. <a href="#">data</a> Zenodo Code used to analyse mortality data from 24 countries. <a href="#">code</a> Zenodo
<b>Proteome profiling of home-sampled dried blood spots reveals proteins of SARS-CoV-2 infections</b> Fredolini C., Dodig-Crnković T., Bendes A., Dahl L., et al (2024) Springer Science and Business Media LLC DOI: 10.1038/s43856-024-00480-4	Protein levels obtained from dried blood spot (DBS) samples. <a href="#">data</a> Figshare Data from multiplexed serology assays to determine IgG and IgM levels against several versions of SARS-CoV-2 proteins. Samples obtained from dried blood spots (DBS). <a href="#">data</a> Figshare Code for the analysis and visualisation of proteome data from home-sampled dried blood spots. <a href="#">code</a> GitHub

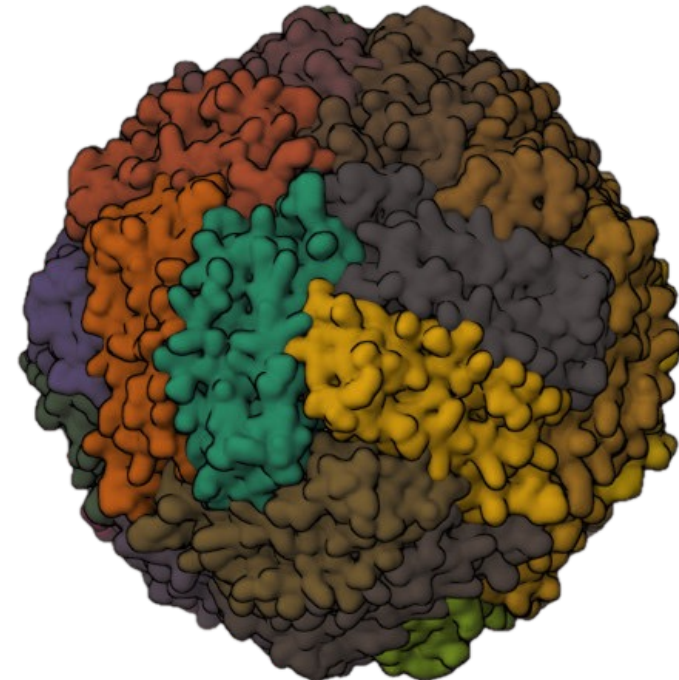
<https://www.pathogens.se>

# 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	😞	😊

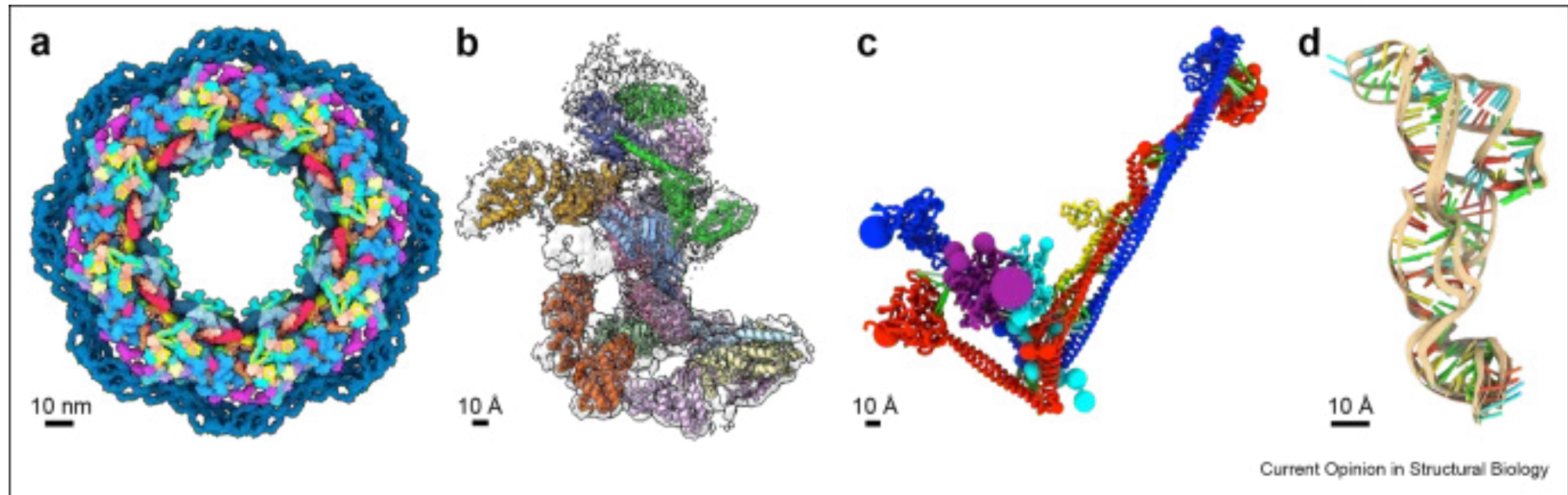




# New systems



- 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?

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Well-curated data sets

Cutting edge science

Access to cross-platform and cross-facility experiments

Long-term: closer collaboration with healthcare



SANS can be used to showcase the approach

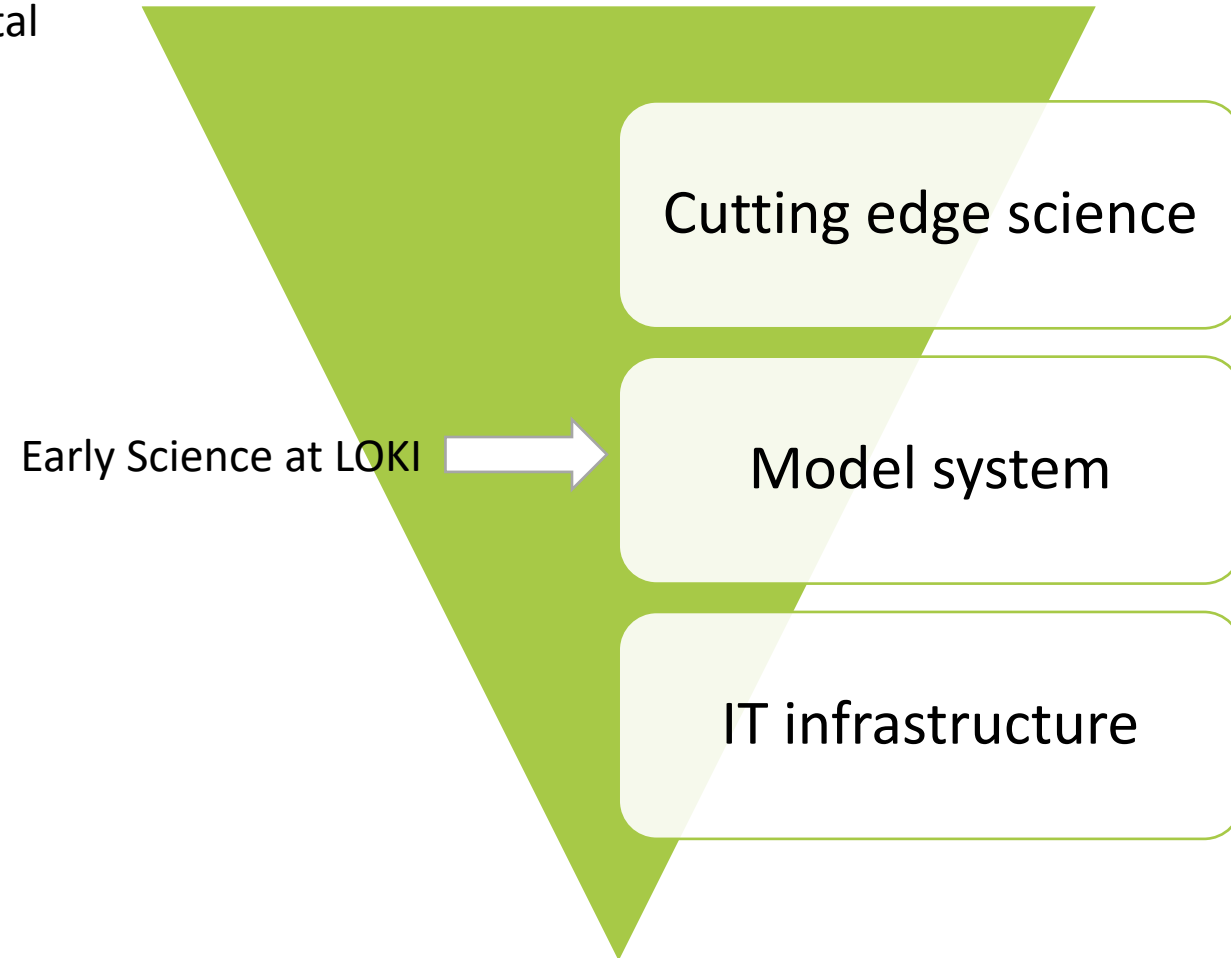
Well-characterized biological systems for instrument debugging (including SEC-SANS)

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



## Visit us:

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