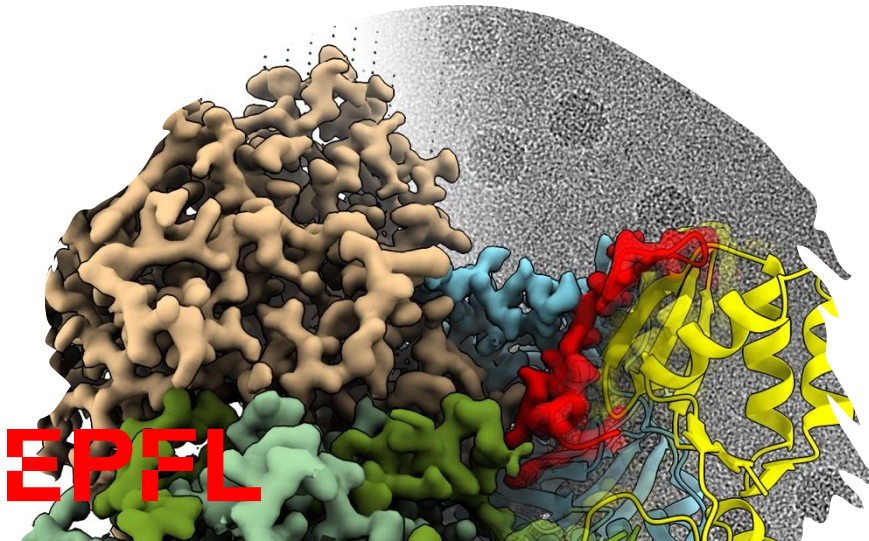


EDMS BIO-643: Integrative Structural Biology for Life Sciences

- Luciano Abriata
- Kelvin Lau
- Yoan Duhoo
- Anna-Sophia Krebs
- Jonathan Schneider
- Florence Pojer
- Guest: Prof. Henning Stahlberg

**Protein Production and Structure Core
Facility, SV-PTPSP**

Fall Semester 2025





Course objectives



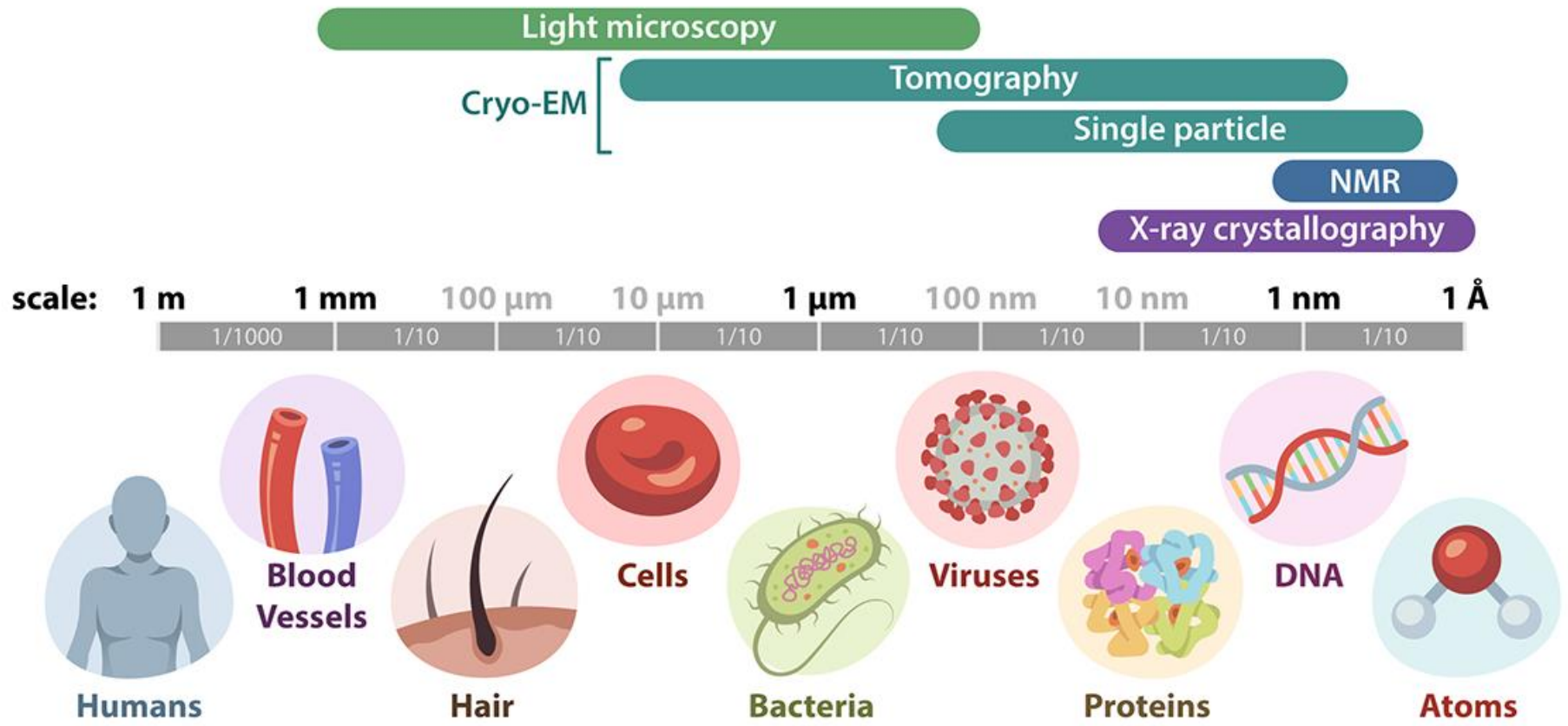
Hands-on on Structural Biology resources, software and techniques, including visualization modeling tools and data obtained by NMR, X-ray crystallography and SPR cryoEM.



Team-based interactive class



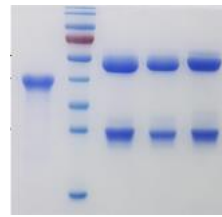
Develop your own analysis and critical interpretation of real data



***In silico* models**

- Alphafold
- Swissmodel
- Rosetta,..

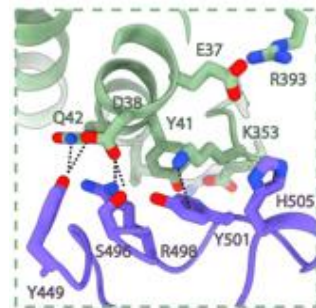
```
MKLTLNLSMAIMMSIVMGS  
SAMAADSNEK...GAS  
GYLPEHTL...  
ADYLEQD...  
LHDHYLD...  
DRARKDG...  
DEIKSLKF...  
QTYPGRFPMG...  
HTFEEIEFVQGLNHSTGK  
NIGIYPEIKAPWPHQEGKDI  
AAKTLEVLKKYGYTGKDDKV
```



X-ray Crystallography

NMR

Single-particle CryoEM

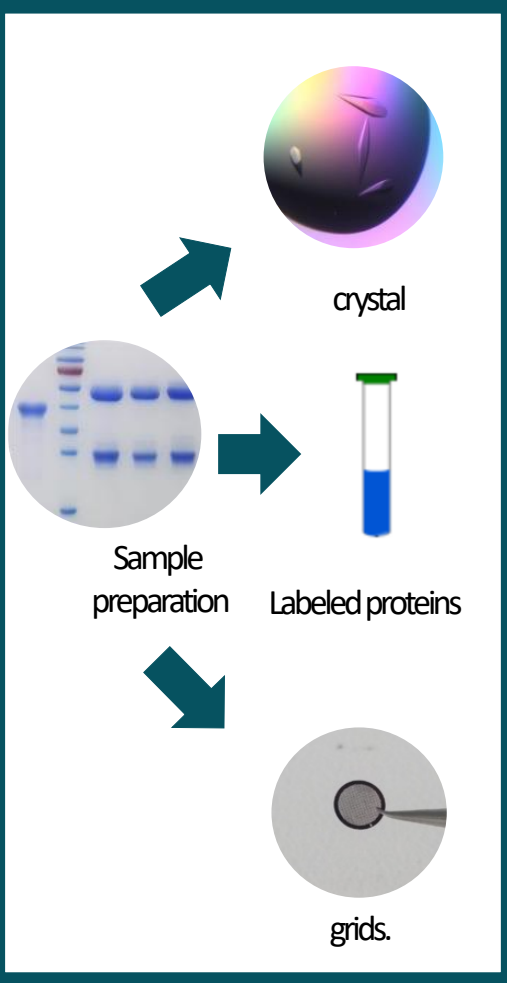


September 2025: 242 066 structures deposited in PDB database

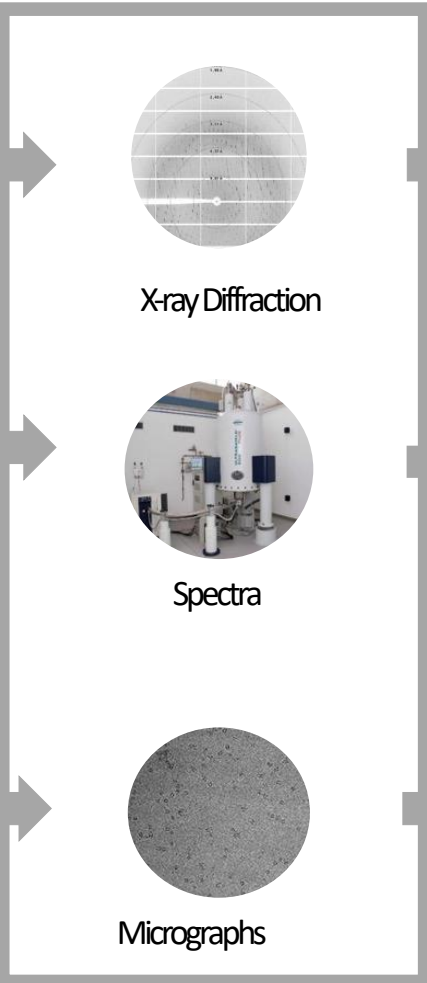
Number of Released PDB Structures per Year

Year	↓	X-Ray	↑	NMR	↑	EM	↑
2025		7,169		153		5,022	
2024		9,206		284		5,791	
2023		9,584		272		4,576	
2022		9,824		301		4,104	
2021		9,238		360		2,951	
2020		11,195		381		2,386	
2019		9,618		380		1,451	
2018		9,853		392		882	
2017		10,067		412		563	
2016		9,922		449		412	

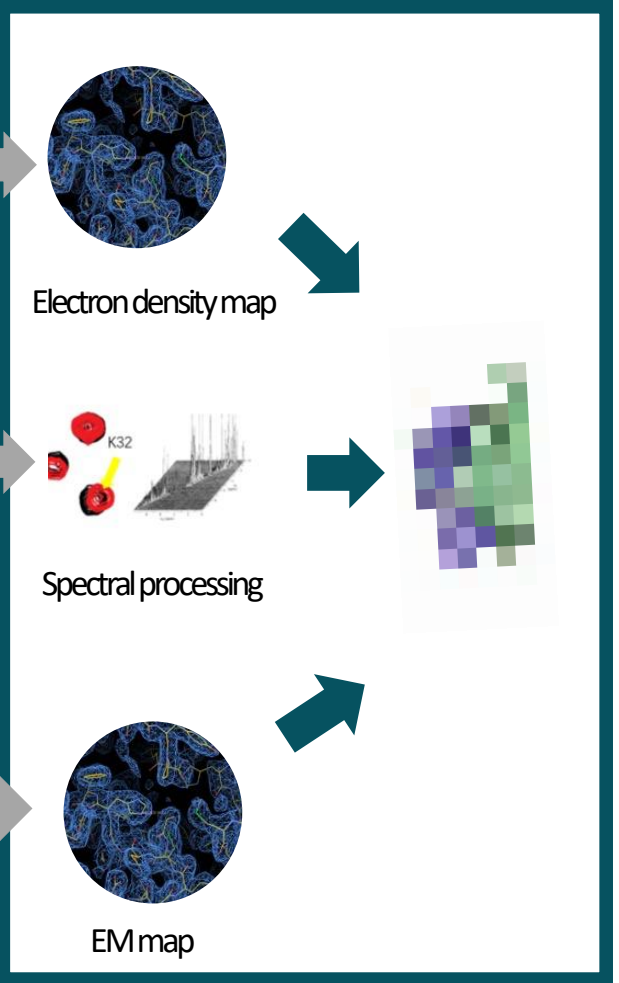
SAMPLE PREPARATION
At PTPSP or labs



DATA ACQUISITION
High-end facilities



DATA PROCESSING to MODEL
At PTPSP or labs



High-ends Facilities to collect Data



NMR FACILITY AT EPFL



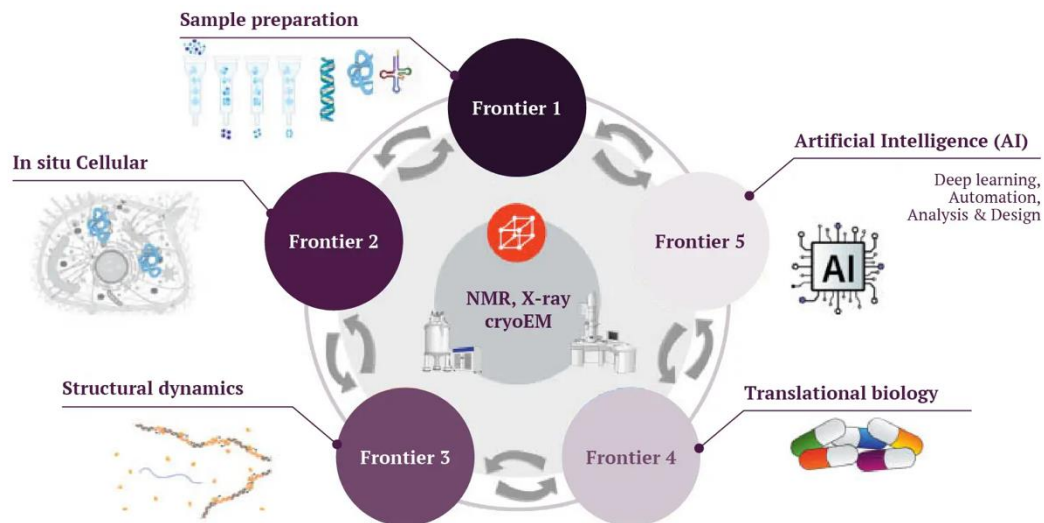
X-RAY SYNCHROTRONS AT ESRF AND SLS



CRYOEM AT DCI EPFL UNIL

How to decide on the method?

- The biological question: nature and size of protein/complexes and type of results wished
- Pros/cons for each method - each project carefully evaluated
- Time and funding
- Expertise and access to technology



	PROS	CONS
X-ray crystallography	<ul style="list-style-type: none"> ✓ Provide very detailed atomic information ✓ Easy to perform ✓ Not expensive ✓ Software free and user friendly ✓ No size limitation ✓ Synchrotron facilities around the world 	<ul style="list-style-type: none"> ✓ Need to form crystals ✓ High protein quantity ✓ Difficult for membrane proteins ✓ Difficult for flexible domains
BioNMR	<ul style="list-style-type: none"> ✓ Small flexible proteins ✓ In solution ✓ Info on dynamics ✓ Info on ligand binding 	<ul style="list-style-type: none"> ✓ Not for big complex. (samples < 40kDa) ✓ Low through-put ✓ High expertise ✓ High protein quantity, labeled ✓ Expensive
Single-particle EM	<ul style="list-style-type: none"> ✓ Big complex, membrane proteins ✓ Not much protein needed (10 times less than crystallography) ✓ Achieve atomic resolution 	<ul style="list-style-type: none"> ✓ Still challenging for small protein < 60kDa ✓ High expertise ✓ Low Throughput ✓ High-end equipment ✓ Expensive

EDMS BIO-643

Integrative structural biology for Life sciences

Fall semester 2025

Date/Time: Thursdays 3:15 to 5pm

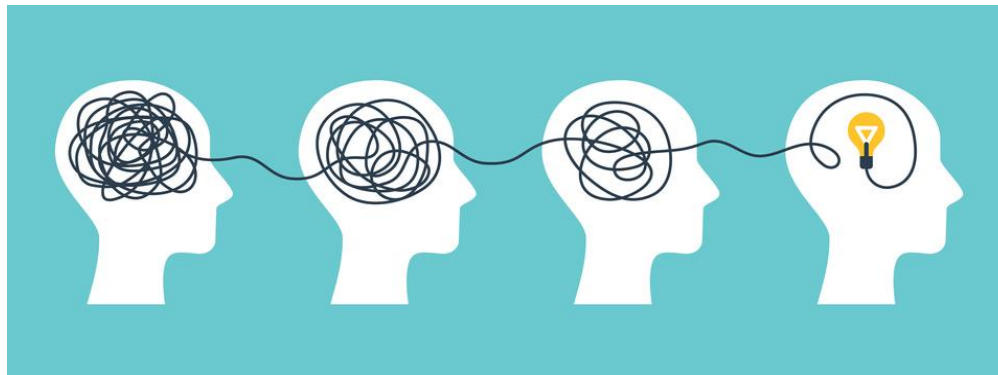
Location: AI 3142

Date	Topics	Speakers
Sept 11th	Course introduction	All teachers
Sept 18th	Modeling tools	Luciano
Sept 25th	Modeling tools -visualization in ChimeraX	Luciano, Yoan, Kelvin
Oct 2nd	X-ray crystallography theory + software	Florence/Kelvin
Oct 9th	no class	
Oct 16th	X-ray software	Kelvin/Florence
Oct 23rd	no class (EPFL break)	
Oct 30th	X-ray software	Kelvin/Florence
Nov 6th	cryoEM theory	Prof. Henning Stahlberg
Nov 13th	cryoEM software	Yoan, Anna-Sophia, Jonathan
Nov 20th	cryoEM-ET software	Yoan, Anna-Sophia, Jonathan
Nov 27th	cryoEM-ET software + visit DCI	Yoan, Anna-Sophia, Jonathan
Dec 4th	Bio-NMR theory + software + visit	Luciano, Kelvin
Dec 11th	Students presentations	All teachers
dec 18th	Students presentations	All teachers

Evaluation - Presentation

LEARN FROM EACH OTHER EXPERTISE AND BACKGROUND

- Organize group of two to three students
- Each group pick a paper with structural data and communicate it to teachers
- Goal: to analyse the structural data included in the chosen paper and emphasize the techniques including the raw data
- Present the data in an interactive way to your colleagues and teachers
- 20 mins presentation + 10 mins Q&A
- Be critical against the data, the results and their interpretations



Bio-643 Moodle

<https://moodle.epfl.ch/>

Resources needed for the course

[Bio-643 protein structures resources and software](#)

Deposition database for all structures

[PDB Database](#)

Any questions?

Let's install all the software on your laptop and check they are working properly