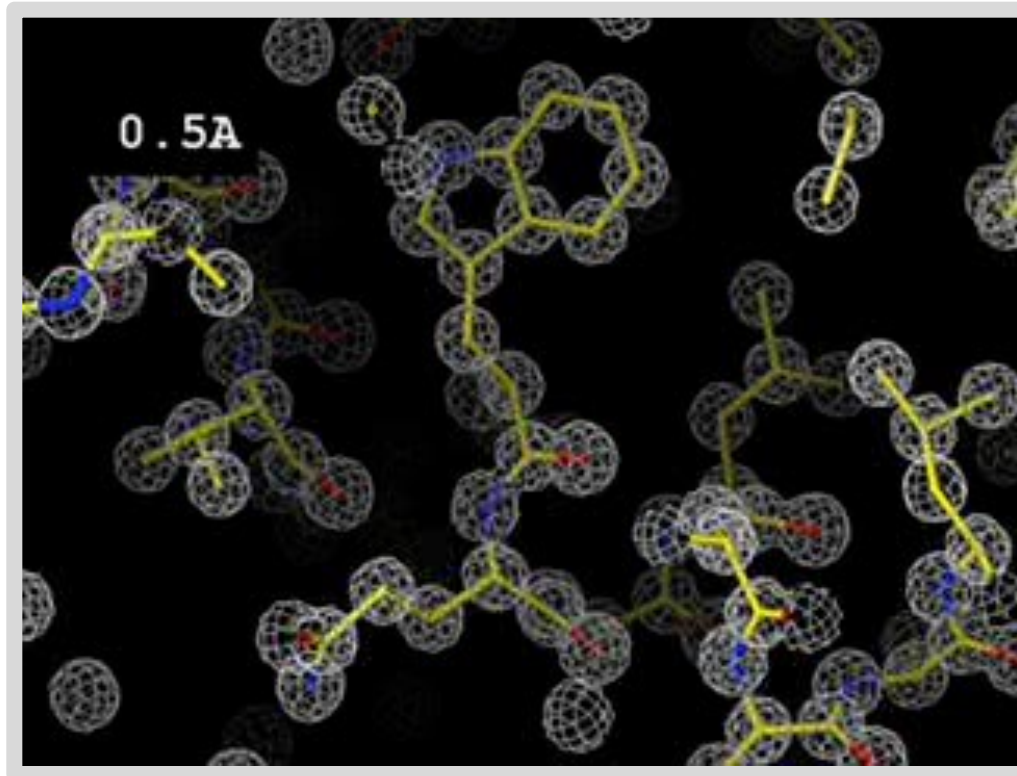


EDMS BIO-643: Integrative Structural Biology for Life Sciences



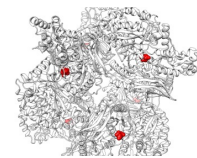
Luciano Abriata

Kelvin Lau

Yoan Duhoo

Florence Pojer

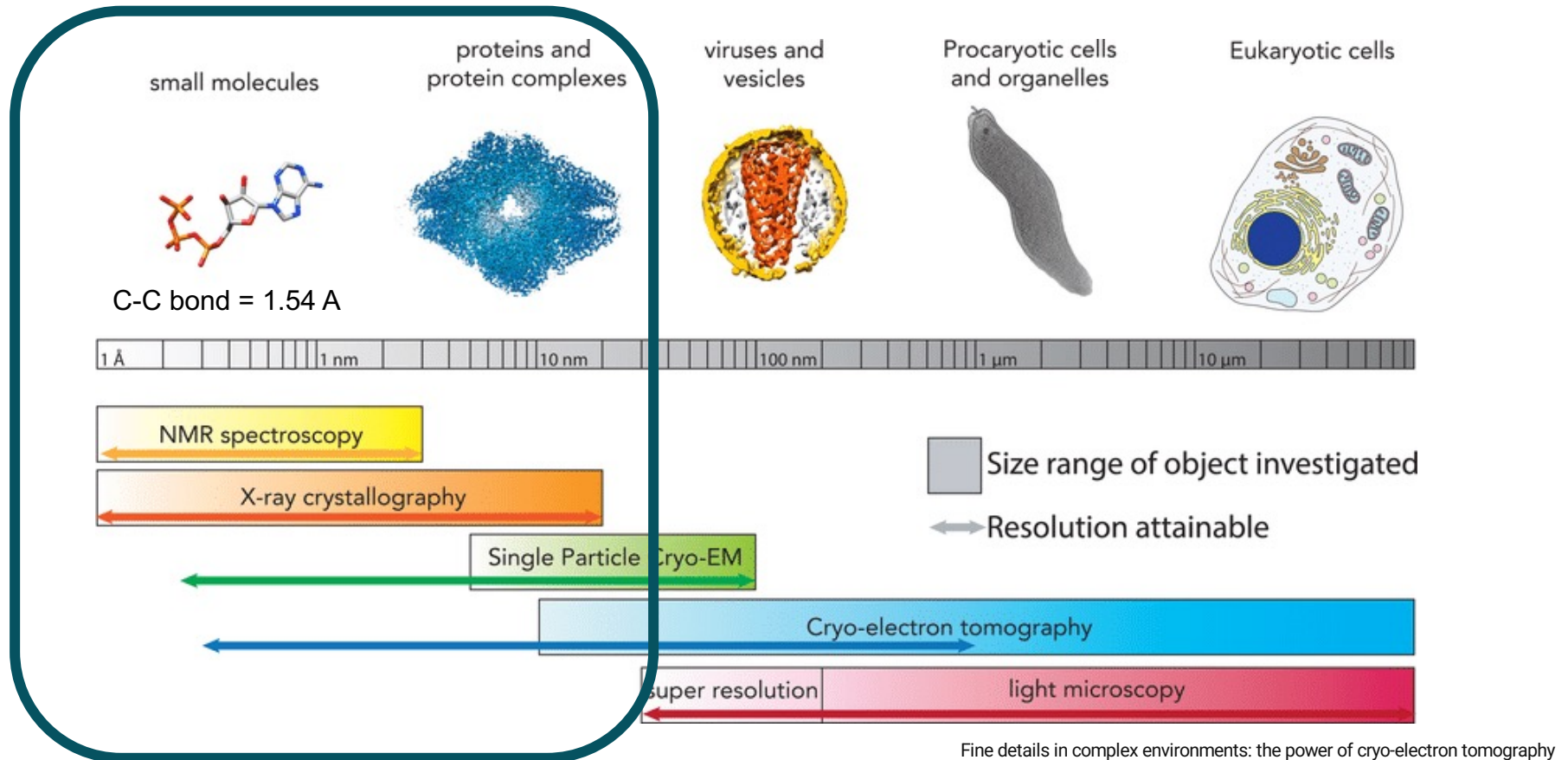
Protein Production and Structure Core Facility, SV-PTPSP

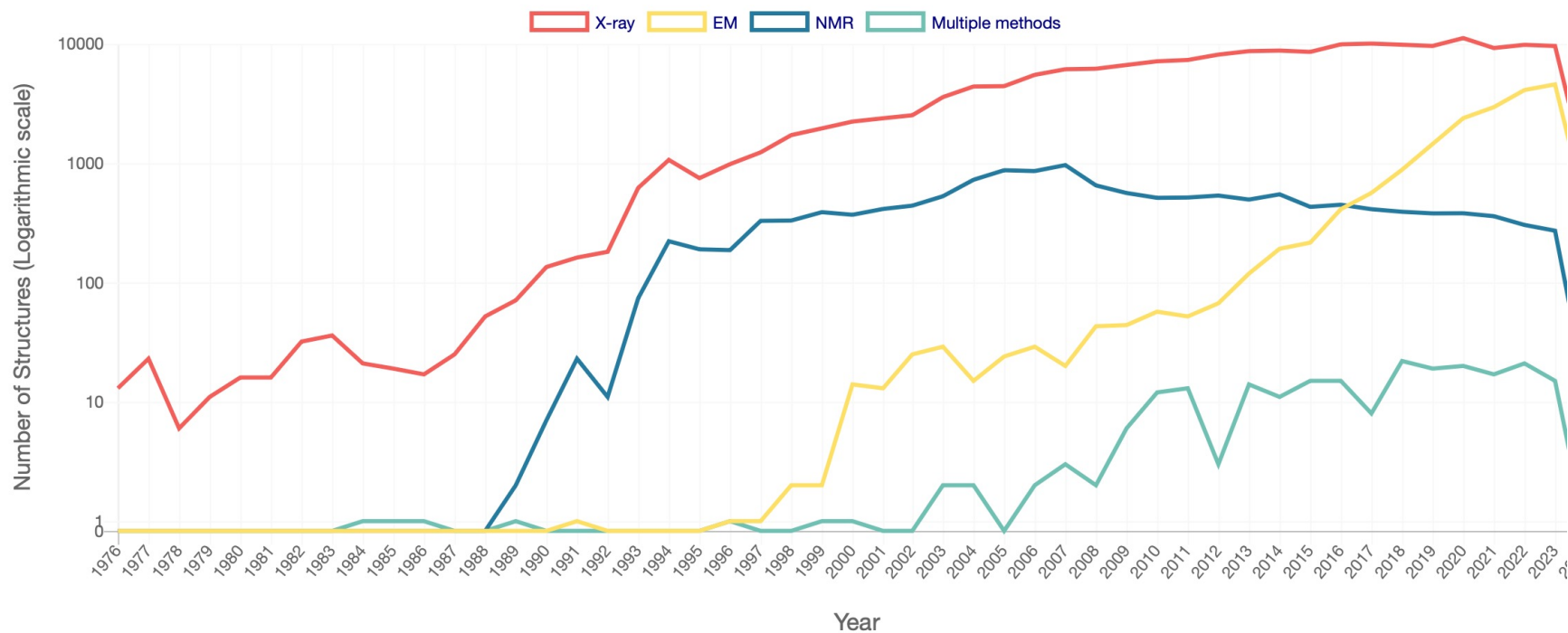


Course goals

- 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

Tools for Structural characterization



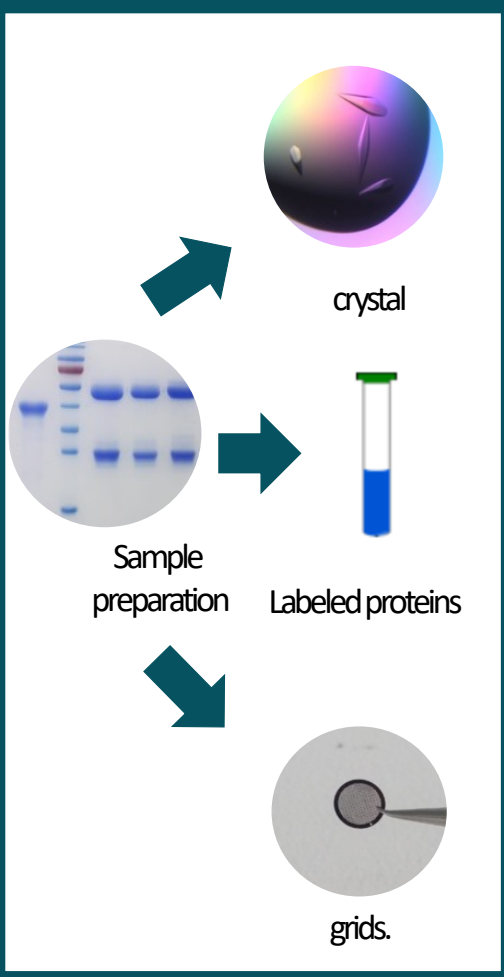


Year	↕	X-Ray	↕	NMR	↕	EM	↕
2024		854		13		415	
2023		9,615		272		4,582	
2022		9,833		304		4,109	
2021		9,242		360		2,952	
2020		11,197		381		2,387	
2019		9,622		380		1,451	
2018		9,853		392		882	
2017		10,071		412		564	
2016		9,927		449		412	
2015		8,578		431		216	

<https://www.rcsb.org/stats/all-released-structures>

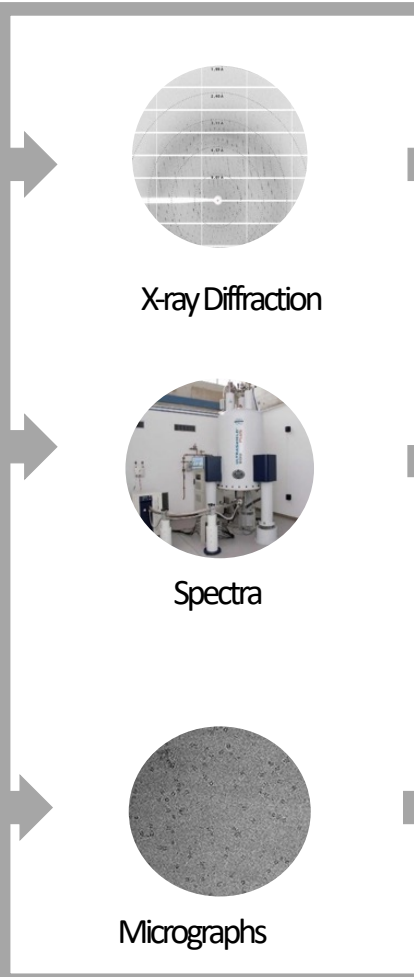
SAMPLE PREPARATION

At PTPSP or labs



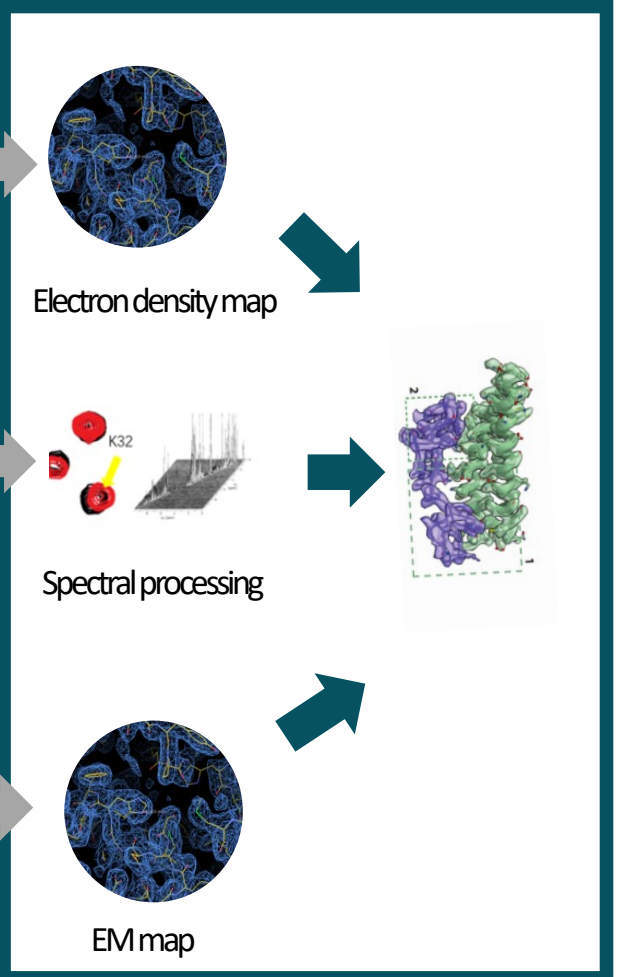
DATA ACQUISITION

High-end facilities



DATA PROCESSING to MODEL

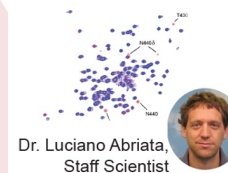
At PTPSP or labs





Close contacts to High-end facilities

Bio-NMR
@ NMR facility, EPFL



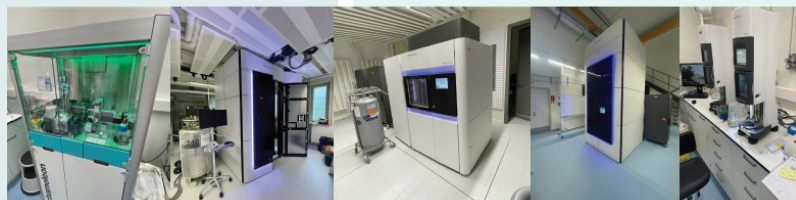
Dr. Luciano Abriata,
Staff Scientist

X-ray Crystallography
@ SLS PSI, Villigen



Dr. Kelvin Lau,
Staff Scientist

SPR, CryoEM
@ DCI, join EPFL,
UNIL & Uni Geneva



Dr. Yoan Duhoo,
Staff Scientist



Advice: How to decide the methods

To consider:

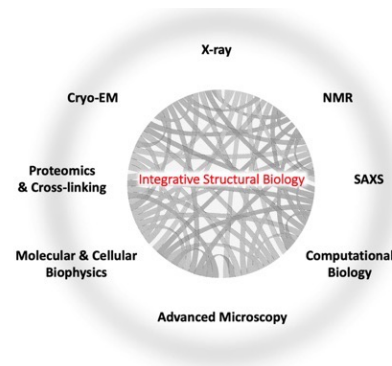
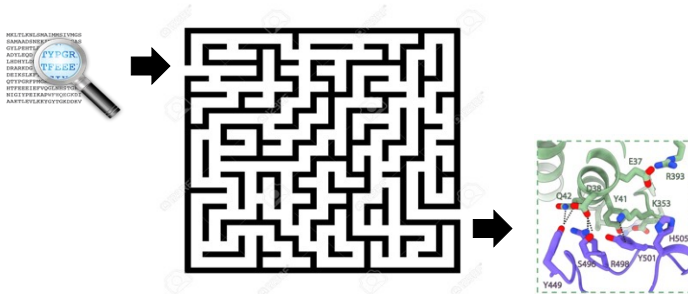
❑ The Biological question: nature and size of proteins/complexes and type of results wished

Pros/cons for each method. Each project is evaluated carefully.

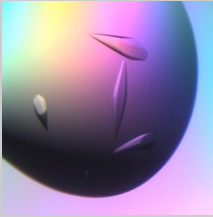
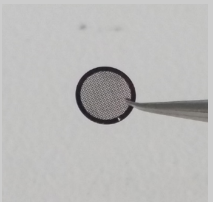
Roughly: SPR cryoEM for proteins > 60kDa & big complexes & difficult to produce; NMR for small flexible proteins < 40kDa; crystallography for drug target & protein any size; but with limiting factor being the formation of crystals

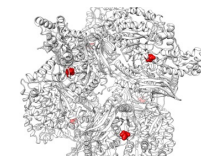
❑ Time and funding

❑ Expertise and access to technology



- ✓ Methods complement each other
- ✓ Often performed in parallel

Techniques	PROS	CONS
X-ray crystallography 	✓ Provide very detailed atomic information ✓ Easy to perform ✓ Not expensive ✓ Software free and user friendly ✓ No size limitation ✓ Synchrotron facilities around the world	✓ Need to form crystals ✓ High protein quantity ✓ Difficult for membrane proteins ✓ Difficult for flexible domains
BioNMR 	✓ Small flexible proteins ✓ In solution ✓ Info on dynamics ✓ Info on ligand binding	✓ Not for big complex. (samples < 40kDa) ✓ Low through-put ✓ High expertise ✓ High protein quantity, labeled ✓ Expensive
Single-particle EM 	✓ Big complex, membrane proteins ✓ Not much protein needed (10 times less than crystallography) ✓ Achieve atomic resolution	✓ Still challenging for small protein < 60kDa ✓ High expertise ✓ Low Throughput ✓ High-end equipment ✓ Expensive



Schedule

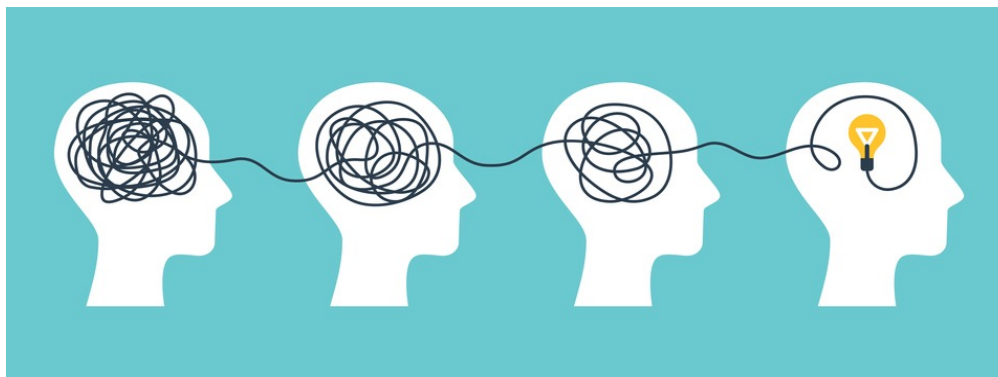
Date	Topics	Speakers
Feb 19th	Course introduction	Florence/Luciano/ Kelvin/Yoan
Feb 26th	Modeling tools	Luciano
March 4th	Modeling tools	Luciano
March 11th	X-ray crystallography theory + software	Florence/Kelvin
March 18th	X-ray software	Kelvin/Florence
March 25th	X-ray software	Kelvin/Florence
April 1st	no class	
April 8th	cryoEM theory + software	Yoan/Kelvin/Florence
April 15th	cryoEM software	Yoan/Kelvin/Florence
April 22th	cryoEM software	Yoan/Kelvin/Florence
April 29th	Bio-NMR theory + software	Luciano
May 6th	Bio-NMR software	Luciano
May 13th	Bio-NMR software	Luciano
May 20th	Students presentations	
May 27st	Students presentations	

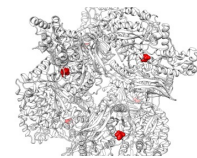


Evaluation - Presentation

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

<https://go.epfl.ch/bio-643>

Deposition database for all structures

[PDB Database](#)

Any questions?

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

<http://labriataphd.altervista.org/struct-biol-course/spring2022.html>