

CH-609

Introduction to the ChemInfo ELN of ISIC

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
Hours	21
Lecture	7
Project	14
Number of positions	

Frequency

Only this year

Remark

October 10th 2022

Summary

This course will be on Electronic Laboratory Notebooks and is aimed at (future) users. Multiple electronic lab notebooks exists. The course will focus on the Cheminfo tools (<https://eln.epfl.ch/>).

Content

Pre-workshop assignment

- Documentation of current research data management and research workflow (what data are generated, how are they analyzed, stored, and backed up)
 - What are the current bottlenecks and pain-points
 - What works well?
 - Fill pre-workshop survey
 - User story of how the ELN should look like
- Workshop (10.10.2022, in person in Sion)
- Introduction to the cheminfo ecosystem:
 - Philosophy
 - Store/retrieve original data
 - Extract knowledge
 - Publish machine actionable data
 - Overview of existing tools in the cheminfo ELN (image analysis, mass spec, ML, XRD, isotherm, export, TGA, etc)
 - Deep dive into three tools available in the cheminfo ELN
 - Interactive discussions:
 - What is missing?
 - What does not work?
 - What would be the best support mechanism?

Post-Workshop

- Submit feature requests, bug reports, ideas

Keywords

electronic laboratory notebooks

Learning Prerequisites**Required courses**

Basic thermodynamics and some basic knowledge on computational methods (e.g., Matlab or programming)

Learning Outcomes

By the end of the course, the student must be able to:

- Make chemical data machine actionable.
- Use ELNs to store and retrieve data,

Resources

Bibliography

Jablonka, K. M.; Patiny, L.; Smit, B. Making the Collective Knowledge of Chemistry Open and Machine Actionable.

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the Flow of Your Data from the Magnet to the Public. Magnetic Resonance in Chemistry 2018, 56 (6), 520-528.

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