

# ChE-601 Hands-on with Research Data Management in Chemistry

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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	24
Courses	12
Exercises	3
TP	9
Number of positions	15

## Frequency

Every year

#### Remark

Next time January 2022

## **Summary**

PhD students in Chemistry will learn hands-on Research Data Management (RDM) skills transferable to their research practices. They will contextualize their research into RDM best practices (day 1), discover appropriate tools (day 2) and work on a project (day 3) for the course accreditation

#### Content

# **DAY 1: RDM GOOD PRACTICES & EPFL SOLUTIONS**

Main scope: PhD students will contextualize their current lab RDM practices in light of FAIR principles

- Contextualize the FAIR data principles in the chemical research field
- Discover the SNSF DMP as a guideline
- Differentiate between raw data, processed data and code
- Compare ELNs and other collaborative solutions
- Collaborative tools:
- --- Collaborative writing tools (Authorea, Overleaf, HackMD, ...)
- --- Electronic Lab Notebooks (EPFL ELN, SLIMs, OpenBis, ...)
- --- Cloud storage solutions (Switch, EPFL GDrive, OwnCloud, ...)
- Data organization, file naming and documentation
- Discover metadata for research data

### **DAY 2: TOOLS HANDS-ON**

Main scope: PhD students will discover software and platforms to improve their current RDM practices

- Data formats, exporting & conversion
- Differentiate between storage, back-up and preservation solutions
- Data reuse:
- --- Discover the re3data.org
- --- Data access & re-use from data repositories
- Versioning:
- --- Git
- Data manipulation
- --- Dataviz for publication
- --- Open tools for data analysis
- --- Data formats converters

Practical session: PhD students will model and present their current practices and workflows involving research data



### **DAY 3: PROJECT**

Main scope: PhD students will discover further tools and concepts to plan their RDM activities and improve their research workflows

- Dealing with sensitive data, proprietary data and licensing
- Data publishing via data repositories, data archiving
- Computational chemistry workflows and tools

Practical session: PhD students will refine their workflow models and present them for peer-assessment and evaluation

- Pitch the RDM aspects of the research project
- Describe data generation & reuse
- Select relevant and applicable solutions for their project, such as:
- --- storage & collaborative tools
- --- documentation & metadata standards
- --- repositories for data publication and archiving

### **Learning Outcomes**

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

- Define Data Life-Cycle of his/her research
- Identify Specific softwares
- Apply RDM good practices