

ChE-601

**Hands-on with Research Data Management in Chemistry**

Borel Alain, Gabella Chiara, Varrato Francesco

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
<b>Hours</b>	<b>24</b>
Courses	12
Exercises	3
TP	9
<b>Number of positions</b>	<b>15</b>

**Frequency**

Every year

**Remark**

Next time Winter 25 (block)

**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

**Resources****Moodle Link**

- <https://go.epfl.ch/ChE-601>