

CH-801

Big data and machine learning for chemistry

Corminboeuf Clémence

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Written
Workload	30h
Hours	17
Courses	14
Exercises	3
Number of positions	

Remark

June 7 - 9 2021

Summary

An overview of the main concepts and tools of big data, automatisation, and applications of AI in chemistry is presented through lectures and workshops. Specific applications of machine learning to computational chemistry, catalysis, and high-throughput screening are discussed from theoretical, exper

Content**Keywords**

Big Data, machine learning, high-throughput screening, computational chemistry, catalysis

Resources**Websites**

- <https://bdmlc2021.epfl.ch>