



Course unit English denomination	Notions of Machine Learning for Chemistry
Teacher in charge (if defined)	POLIMENO Antonino
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	01-02/2025
Course delivery method	<input checked="" type="checkbox"/> In presence <input type="checkbox"/> Remotely <input type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (50 % minimum of presence) <input type="checkbox"/> No
Course unit contents	Chemistry and data Kernel ridge methods Artificial neural networks methods Genetic algorithms
Learning goals	<p>Knowledge: the aim of the course is to expose the students to modern chemical informatics, machine learning and artificial intelligence driven approaches for computational modelling and prediction</p> <p>Skills: the focus will be on teaching students how to use machine learning algorithms and techniques to analyse and make predictions about chemical data</p> <p>Competencies: the course will cover topics such as the basics of machine learning, common algorithms, and their applications in chemistry.</p>
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers



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Prerequisites (not mandatory)	Basic mathematics/physics/chemistry knowledge acquired in fundamental courses (chemistry/ industrial chemistry/ material sciences) The course does not require any advanced programming skill.
<b>Examination methods</b>	Students will be asked to apply their acquired knowledge to a real-world problem in chemistry, by devising a short research project and applying in practice a machine learning method to solve it. Students will work individually or in small groups to complete their projects. They will prepare and submit a written report, which will summarize the objectives, methods, and results of their case studies. A discussion will conclude the assessment, based on both the report and the general understanding of the fundamental principles of Machine Learning applied to chemistry
Study material	Slides/articles provided by the teacher
Additional information (not mandatory)	Hands-on sessions will accompany lecture activities, to provide the students with practical guidelines on how to perform simple machine learning experiments for real case studies in chemistry, performed with Python-based tools.

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