



MINISTERIO  
DE CIENCIA, INNOVACIÓN  
Y UNIVERSIDADES



The Vice-Presidency for Scientific and Technical Research of the Spanish  
National Research Council (CSIC) certifies to:

**Caroline Coxwell Mohler**

with passport number 680618731  
for having studied and passed in Jaca (Huesca), from 16 to 19 June 2024,  
the MICROCREDENTIAL in:

***Cheminformatics, automation, and machine learning in chemistry: from  
fundamental concepts to emerging techniques***

organized by the Institute of Chemical Synthesis and Homogeneous Catalysis  
of the CSIC, with a duration of 25 hours and in which, by means of evaluation,  
has reached the adequate degree of learning whose objectives  
and contents are shown on the back.

The vice-president

José María Martell Berrocal



Financiado por la Unión Europea  
NextGenerationEU



Plan de Recuperación,  
Transformación  
y Resiliencia



CSV : GEN-ba12-9d7f-1c56-d9f3-34e0-0a4e-fc39-9a9a

DIRECCIÓN DE VALIDACIÓN : <https://sede.administracion.gob.es/pagSedeFront/servicios/consultaCSV.htm>

FIRMANTE(1) : JOSE MARIA MARTELL BERROCAL | FECHA : 18/07/2024 10:32 | Sin acción específica





**OBJECTIVES:** train computational chemists in the use and development of emerging digital technologies in chemistry by combining the basic concepts of machine learning to broaden their knowledge of machine learning, automation and chemoinformatics.

### CONTENTS:

- Python and its scientific modules.
- Intro to SMILES, RDKit & OpenBabel.
- Current advances on cheminformatics.
- Advanced round table discussions I.
- Advanced round table discussions II.
- C REST and conformational searches.
- Q&A of day 1.
- Open source in comp. chem.
- Automation of QM with AQME.
- ML in chemistry.
- Intro to chemical ML.
- Q&A of day 2.
- ML automation with ROBERT.
- Automation of custom workflows.

