



MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES



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

Md Bin Yeamin

with foreign identification number Y25I634IV
for having studied and passed in Jaca (Huesca), from 16 to 19 June 2024,
the MICROCREDENTIAL in:

Y25I634IV

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,

The vice-president

José María Martell Berrocal



Financiado por la Unión Europea
NextGenerationEU



Plan de Recuperación,
Transformación
y Resiliencia





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.

