



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

## Md Bin Yeamin

with foreign identification number Y2516341V for having studied and passed in Jaca (Huesca), from 16 to 19 June 2024, the MICROCREDENTIAL in: Y2516341V

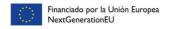
for having studied and passed in Jaca (Huesca), from 16 to 19 June 2024, the MICROCREDENTIAL in:

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













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 I.
- 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.

