

## **Intelligent modeling and classification of NMR spectroscopic data**

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This poster presents the research project of my Cifre thesis at Evear extraction in partnership with University of Lyon 1, on the modeling and intelligent classification of NMR spectroscopic data, utilizing a 400MHz NMR spectrometer and AI models trained on 4 Nvidia L4 GPUs. The main goal is to develop a metric for comparing two NMR spectra, enabling rapid and precise detection of similarities. This approach facilitates the identification of components in complex samples which would associate each peak in the NMR spectrum with a specific molecule. Particular attention is given to the classification of plants from their NMR spectra, aiming to specifically identify the studied plant among a defined set. This methodology relies on detecting the unique characteristics present in each spectrum, allowing for accurate recognition of the molecules comprising the sample. Early results on a machine learning workflow based on a random forest algorithm will be presented. This project promises to significantly improve the speed and accuracy of chemical compound identification, offering potential applications in various scientific and industrial fields. It represents a notable advancement in the use of NMR spectroscopy, opening new perspectives for the exploration of spectroscopic data in research and beyond.

**Keywords:** NMR, AI, Metabolomics