



Contribution ID: 4

Type: **Presentation short (15 min)**

## **Implementation of FAIR principles in nuclear magnetic resonance (NMR) spectroscopy experimental workflows**

*Tuesday, 19 October 2021 11:45 (15 minutes)*

Over the past decades, the scientific domain has seen an exponential growth of data generation. As expected, the storage, management and analysis requirements are growing proportionally, with a direct impact on the scientific output. Certain scientific communities like the astronomical one, have already organised and standardised computational workflows, whereas others can benefit from modern good practice principles. These are called FAIR principles and are currently actively supported by the ecosystem of the European Open Science Cloud (EOSC).

This contribution presents the ongoing activities regarding the implementation of FAIR principles in a Nuclear Magnetic Resonance (NMR) spectroscopy experimental workflow, performed at the CERIC-ERIC partner facility, NMR centre at the National Institute of Chemistry (Slovenia). The experiments carried out at this facility range from biological and pharmaceutical studies to studies in energy and basic matter research of high impact. The complete data life cycle has been upgraded, including new approaches to data and metadata acquisition, storage, archiving, processing and visualisation through web and cloud services, paving the way towards advanced data science on the measured datasets. Furthermore, integration of the entire pipeline into the open-source Jupyter web services is also in development. The goal is fostering cross-discipline open science while improving efficiency and accessibility. This is done in the context of a major EU project (PaNOSC) that connects six European large-scale research centres and two e-infrastructures, providing photon- and neutron-based analytical techniques.

The reported results outline certain challenges encountered during the conceptualization and implementation of the NMR workflow upgrade, e. g. handling experimental data from offline devices. At the same time, the aim for the results is to be useful to other scientific fields in the process of adopting FAIR principles and more efficient data handling, tracking and processing.

Speaker bio: <https://www.linkedin.com/in/aljosa-hafner-99350b174/>

### **Most suitable track**

Collaborating across boundaries

**By submitting my abstract, I agree that my personal data is being stored in accordance to conference Privacy Policy**

**Primary author:** HAFNER, Aljosa (CERIC-ERIC - Central European Research Infrastructure Consortium)

**Co-authors:** IPPOLITI, Matteo (Elettra Sincrotrone Trieste); DE SIMONE, Marco (CERIC-ERIC); COGHETTO, Emiliano (CERIC-ERIC); LORENZON, Andrea (CERIC-ERIC); OLIVO, Alessandro (CERIC-ERIC); PODBEVSEK, Peter (Slovenian NMR Centre, National Institute of Chemistry); SKET, Primoz (Slovenian NMR Centre, National Institute of Chemistry); KOUROUSIAS, George (Elettra Sincrotrone Trieste)

**Presenter:** HAFNER, Aljosa (CERIC-ERIC - Central European Research Infrastructure Consortium)

**Session Classification:** Collaboration Accross Boundaries - Presentations

**Track Classification:** Collaboration Accross Boundaries