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Design of metadata schemas for ion chromatography in applied plasma sciences

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Ion chromatography (IC) is an analytical method that separates ions in liquid samples according to their chemical and physical properties. This analytical method is widely used in different scientific fields such as environmental science (for example wastewater or soil analysis), food technology (food extract analysis), applied plasma science (characterization of plasma treated liquids) and protein purification.

To date publications often lack method-relevant parameters, such that a full adaptation of the published methods is not possible. This requires additional testing and hinders the reuse and comparison of methods for IC. We observe that no open, standardized metadata schema exists for IC and related analytical methods, e.g. for high-performance liquid chromatography and gas chromatography. Therefore, we propose a standardized metadata schema to increase the interoperability and reproducibility of scientific investigations in IC. The metadata schema furthermore is a step towards introducing the FAIR principles to the scientific community as a starting point to discuss modern practices in scientific research data management.

This work focuses on the design of two standardized metadata schemas, one for anions and one for cations. These schemas built upon the JSON standard, which sets rules and guidelines for the structure and format of JSON files. Their design is based on the ASTM E 1151 norm for terms and relationships in IC and user-feedback resulting from a coupled data stewardship in applied plasma science. Both schemas are similar in structure and contain relevant metadata for the description of the instrument method (the device settings), processing method (detection windows for automatic labeling of peaks), sample parameters, column properties, quality assurance parameters. Differences are in the specific fields, e.g. different columns for anions/cations and the definition of detection windows for the peak labeling is different. The mandatory fields according to the DataCite metadata schema v4.4 are used for publishing data in repositories and for data citations.

The metadata schemas were designed and tested in a laboratory workflow at the INP with a research data management tool called Adamant [1], which is a user-friendly JSON schema based metadata editor. Users without any programming experience can edit and collect metadata in an HTML form, enabling them to properly collect and validate their metadata (a benefit from the JSON schema standard). The presented use-case demonstrates the paradigms of modern research data management for research in the laboratory. The collected metadata can also be sent directly from Adamant to the institute's instance of the electronic lab notebook (ELN) "eLabFTW"[2] to enable a smoother transition from the traditional handwritten laboratory notebooks to a digital solution, which increases both the interoperability and accessibility of the collected metadata. The ELN also allows the further description of the experiments and linkage with other parts of the related experiment, e.g. sample preparation, treatment and data post processing.

- 1. Chaerony Siffa, I., J. Schäfer, and M. Becker, Adamant: a JSON schema-based metadata editor for research data management workflows. F1000Research, 2022.
- 2. Nicolas Carpi, A.M.a.M.P., eLabFTW: An open source laboratory notebook for research labs. The Journal of Open Source Software, 2017.

Please assign your contribution to one of the following topics

Metadata annotation and management close to the research process

Please specify "other" (stakeholder)

In addition please add keywords.

Research data management, ion chromatography, FAIR principles

Please assign yourself (presenting author) to one of the stakeholders.

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