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# FAIRification of Mass Spectrometry Workflows Using Nanopublication-Based FDOs

## From Specification to Implementation

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**Abstract.** Mass spectrometry research confronts challenges endemic to data-intensive science: vendor-specific proprietary formats from multiple instruments, complex multi-consortium governance, and the near-impossibility of tracking provenance across thousands of heterogeneous digital objects spanning clinical samples, instrument logs, processing workflows, and publications. We address these systemic challenges in the Metabolomics and Analytics Center (MAC) of Leiden University, a high-throughput mass spectrometry laboratory, by implementing nanopublication-based FAIR Digital Objects (FDOs) as minimal, type-specific "metadata tags" at the source. Our FDO implementation allows facile creation of novel FDO types as needed that establish unambiguous provenance chains for any object created in the workflow. The FDO templates are openly available for reuse by anyone and provide the precise context required by agentic systems.

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## 1. Background

Following a comparative analysis demonstrating structural congruence between the Nanopublication Framework and emerging FDO specifications at the First International Conference on FAIR Digital Objects (FDO2022) [1], and a more formal analysis at the Second International FDO Conference (FDO2024) [2], we demonstrated that appropriately designed nanopublications satisfy FDO specification requirements as defined by both the FDO Forum and the FDO Framework. When nanopublication assertions have a persistent link to the object they describe, specify a type, and provide type-specific metadata, they conform to FDO requirements. This established that nanopublications can be deployed as general-purpose "webby" FDO implementations, providing existing infrastructure with substantial FAIR guarantees while minimizing risk of model or vendor lock-in.

## 2. MAC Implementation Strategy

Building on this foundation, we report here operational deployment of nanopublication-based FDOs for FAIRification of mass spectrometry workflows at MAC. Leveraging the FAIR Funder Framework [3]—a generic, minimal, systematic approach enabling research funders to track investments—we developed seven nanopublication-based FDO templates representing core research object types: Research Programme, Call for Proposals, Project, Data Management Plan, Dataset, Method, and Article.

The templates were deployed to create FDO instances in two funded research projects: StayAhead (Health Holland) investigating SARS-CoV-2 variant detection, and Hypermarker (EU) focused on pharmacometabolomic optimization for hypertension treatment. Initially, 14 nanopublication instances were published on NanoDash, providing machine-actionable metadata for research outputs including project descriptions, datasets, analytical methods, and articles. Each instance receives a Trusty URI, timestamp, and cryptographic authentication upon publication from the decentralized Nanopublication Server Network. Once published, these MAC FDOs can be found, discovered, and accessed at open FAIR End Points.

## 3. Technical Approach

The MAC FDO implementation employs a workflow beginning with a Stakeholder Participation Sheet (SPS) that bridges human-machine interaction in template creation. The SPS uses structured notation to guide semantic statement construction, making nanopublication authoring accessible to domain experts without requiring deep RDF expertise. This reduces template creation effort for any digital object type to minimal extensions of a core FDO model. Type-specific metadata includes links to related FDOs in the FAIR Funder Framework, enabling traversal of the complete research object graph via SPARQL queries.

## 3. Results and Impact

The MAC FDO implementation demonstrates that nanopublication-based FDOs operationalize FAIR principles in active real-world research environments, providing infrastructure maturity, scalability, practical utility and interoperability. Current work explores integration with the Dutch National Catalogue and EU Health Data Space. Relevant to industrial applications, the nanopublication approach provides a concrete example of implementing FDOs at scale using existing, stable technologies.

## Data availability statement

All nanopublication-based FDOs used by the Metabolomics and Analytics Center of the Leiden Academic Center for Drug Research are openly available on the Nanopublication Server Network under Creative Commons Attribution 4.0 International https://creativecommons.org/licenses/by/4.0/

## Underlying and related material

NanoDash Project: MAC | Metabolomics and Analytics Center https://w3id.org/kpxl/custom/project/terms/MAC-FDO

## Author contributions

Conceptualization: ES; Methodology & Formal analysis: ES, BM, TK; Investigation: EM, MvdB, AK, AH, TH; Data curation: ES, EM, MvdB; Writing – Original Draft: ES; Writing – Review & Editing: EM, MvdB, AH; Supervision: ES, TH; Funding acquisition: TH

## Competing interests

The authors declare that they have no competing interests.

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## References

[1] Schultes EA, Magagna B, Kuhn T, Suchánek M, Bonino da Silva Santos LO, Mons B (2022). The Comparative Anatomy of Nanopublications and FAIR Digital Objects. Research Ideas and Outcomes 8: e94150. https://doi.org/10.3897/rio.8.e94150

[2] Magagna B, Bonino da Silva Santos LO, Kuhn T, Ferreira Pires L, Schultes E (2024). Nanopublications as FAIR Digital Object Implementations. Open Conference Proceedings 5. https://doi.org/10.52825/ocp.v5i.1417

[3] Bloemers M, Sloep M, Magagna B, Kuhn T, Schultes E (submitted). The FAIR Funder Framework: Implementing Machine-Actionable Research Documentation Through Nanopublication-Based FAIR Digital Objects.