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D4.1 Nanomaterials domain-specific FAIRification mapping

Work Package	WP4 - Nanomaterials
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Abbreviations and Acronyms

API	Application programming interface
ASTM	American Society for Testing and Materials (now ASTM International)
ATP	Adenosine triphosphate (luminometric cytotoxicity assay)
CORDIS	Community Research and Development Information Service
DDI	Data Documentation Initiative
DOIs	Digital Object Identifiers
EChA	European Chemicals Agency
EMMC	European Materials Modelling Council
EMMO	Elementary Multiperspective Material Ontology
EOSC	European Open Science Cloud
FAIR	Findable, Accessible, Interoperable, Reusable
FERs	FAIR Enabling Resources
FIP	FAIR Implementation Profile
FSRs	FAIR Supporting Resources
HEIs	Higher Education Institutions
HTML	Hypertext markup language
IATA	Integrated approaches to testing and assessment
IDs	Identifiers
InChI	International Chemical Identifier
LDH	Lactate dehydrogenase (colorimetric toxicity assay)
NInChI	Nanomaterials International Chemical Identifier
NIKC	Nanomaterials Informatics Knowledge Common

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OECD	Organisation for Economic Cooperation and Development
PARC	Partnership for Assessment of the Risks of Chemicals
PBPK	Physiologically based pharmacokinetic
QMRF	QSAR Model Reporting Format
QSAR	Quantitative Structure-Activity Relationship
REACH	Registration, Authorization and Evaluation of Chemicals
SMILES	Simplified Molecular-Input Line-Entry System
UDS	Uniform Description System on the Nanoscale
VAMAS	Versailles Project on Advanced Materials and Standards

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Executive Summary

WP04 of WorldFAIR aims to increase the FAIRness (Findability, Accessibility, Interoperability and Reusability) of nanomaterials datasets and computational models. The initial focus is on toxicity and safety-related datasets as this is where the bulk of the effort has been to date. We note that nanomaterials are a very broad category of materials, combining chemicals and materials features, and overlapping strongly with the emerging domain of advanced materials. Nanosafety is a very broad domain, covering exposure, toxicity and risk assessment and requires extensive characterisation of the pristine (as-produced) nanomaterials and their physical, chemical, biological and macromolecular transformations within the various environments in which they are present. Thus, the positioning of nanomaterials between Chemistry (WP03) and Geochemistry (WP05) is intentional, as there are strong overlaps of concepts and approaches with both, and solutions applicable to one of these domains are likely to be applicable to others also, leading to the potential for mutual learning and accelerated implementation of the FAIR concepts across these domains.

This specific deliverable lays out the domain and its communities, and the various projects and contributors active in the FAIR-nanomaterials and nanosafety domain. It then presents our initial FAIR implantation Profile (FIP) which describes the current state of the field (an ‘as-is’ FIP) and discusses the domain-specific challenges relating to nanomaterials and its FAIR landscape. The deliverable then lays out the developments needed to reach the ‘to-be’ FIP, as the optimal approach to make nanomaterials and nanosafety data FAIR, based on current best practice across the FAIR community. We note that the As-Is FIP will be updated at the end of the WorldFAIR project, to capture: the rapid development in the field; our own efforts to enhance the number of domain-specific FAIR-enabling Resources (FERs) and FAIR-supporting resources (FSRs); FIPs underway in the aforementioned WorldFAIR Chemistry (WP03) and Geochemistry (WP05) case studies, as well as the efforts underway in the Partnership for Assessment of the Risks of Chemicals (PARC[1]), which has a very strong FAIR data focus. Subsequent activities in WP04 will implement a case study to foster development and piloting of interoperability standards, and guidelines for increasing FAIRness in the interlinked scientific disciplines of chemical toxicity, nanomaterials toxicity and materials modelling.

The FAIR mapping represents a critical step towards identifying both the domain-specific features and the general features needed to maximise nanosafety data and model FAIRness, highlighting areas for further development and standardisation especially in the domain-specific aspects such as metadata standards and ontologies. Existing ontologies have major gaps in their semantic coverage, and project-specific terminology is not fully integrated/accessible via ontology look-up services. Building on the mapping and ‘As-Is’ FIP for nanosafety, WP04 will develop an index (registry) and workflows for FAIRification of nanoinformatics tools and models (D4.2), and recommendations for nanomaterials-specific human and machine-readable provenance and persistence policies (D4.3).

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[1] https://cordis.europa.eu/project/id/101057014

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This nanomaterials FIP, and its subsequent iteration, form a critical part of the overarching WorldFAIR cross-domain mapping and indeed have already been integrated into D2.1 and D11.1.

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1. Nanomaterials and nanosafety assessment

Nanomaterials are defined (for regulatory and related purposes) as materials that have at least one dimension in the nanoscale range (typically less than 100 nanometers). At this size range, they exhibit unique physical, chemical, and biological properties that are different from bulk materials, and from soluble forms such as metal ions. These properties are a result of their high surface area-to-volume ratio, quantum confinement (in some cases), and surface effects, among other factors.

The periodic table, created 150 years ago, is of fundamental importance for various branches of chemistry, physics, and biology as well as being a powerful and precise tool for predictable design of innovative chemical compounds and materials. Indeed, different elements have played critical roles in different periods of human activities, with Silicon (Si) and Lithium (Li) currently being key elements enabling the computer and battery revolutions, respectively.

A recent review by Goodilin et al. (2019) highlights the fact that nanotechnology has brought numerous elements into the limelight (see Figure 1) and transformed their roles in science and technology including s- and p-Block Elements, which are the staples of Energy, Information, and Light technologies, and Pnictogens (the group containing Phosphorus (P) and Nitrogen (N), Group 15); Chalcogens and Halogens, which have critical roles in biomaterials, energy storage, and as smart materials; and Transition Metals (d-block elements) that are widely used in energy devices, sensors, information recording, and nanomedicine.

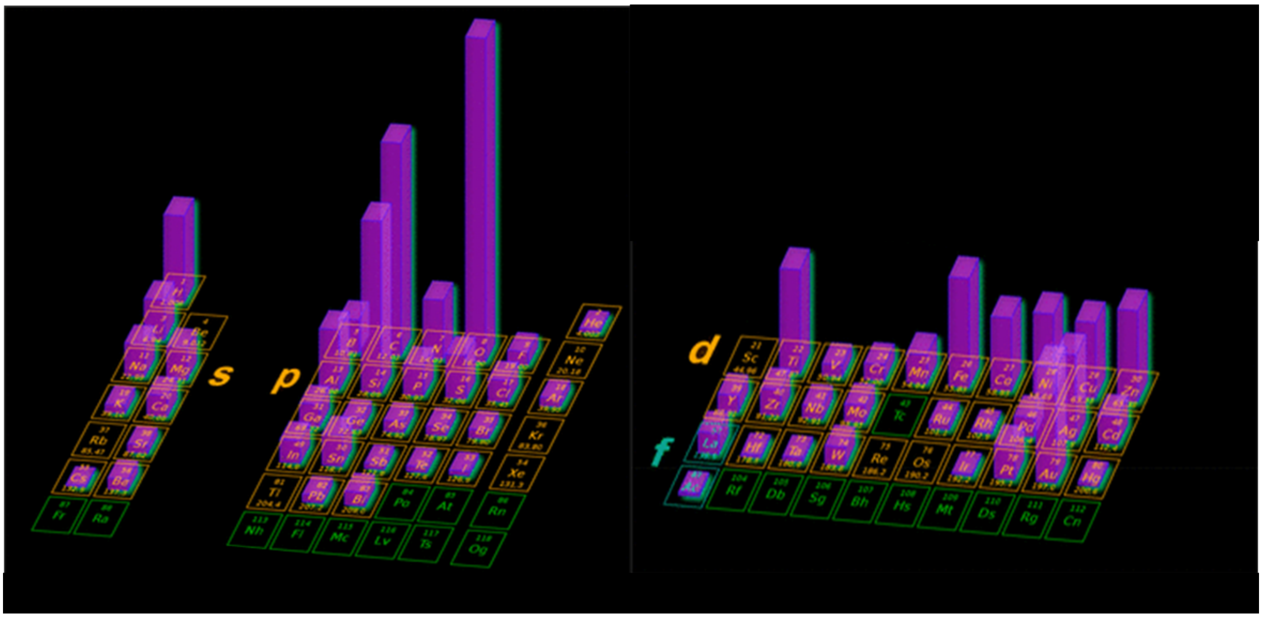

Figure 1. Frequency of usage of chemical elements in nanotechnology, based on analysis by Goodilin et al. (2019) of publications in the journal ACS Nano; higher neon glow bars correlate with the elements'

contribution to the nanotechnology field; green cells denote radioactivity; the f-element families are marked with "La" and "Ac". Notably, ca. 30 of the 118 primary elements that are in high demand for single- and multicomponent nanostructured materials are abundant and inexpensive light elements with large geological resources and reasonable biocompatibility, are chemically inert, or have special redox and crystal chemistry. From Goodilin et al. (2019).

1.1 Nanomaterials as chemicals and particles

Nanomaterials can be considered both chemicals and particles as they exhibit properties of both. They are made up of chemical elements, just like any other chemical substance, and have specific chemical properties that can be studied and manipulated, but they also behave like particles in terms of their size, shape, and behaviour in various environments, including their uptake by organisms and into cells.

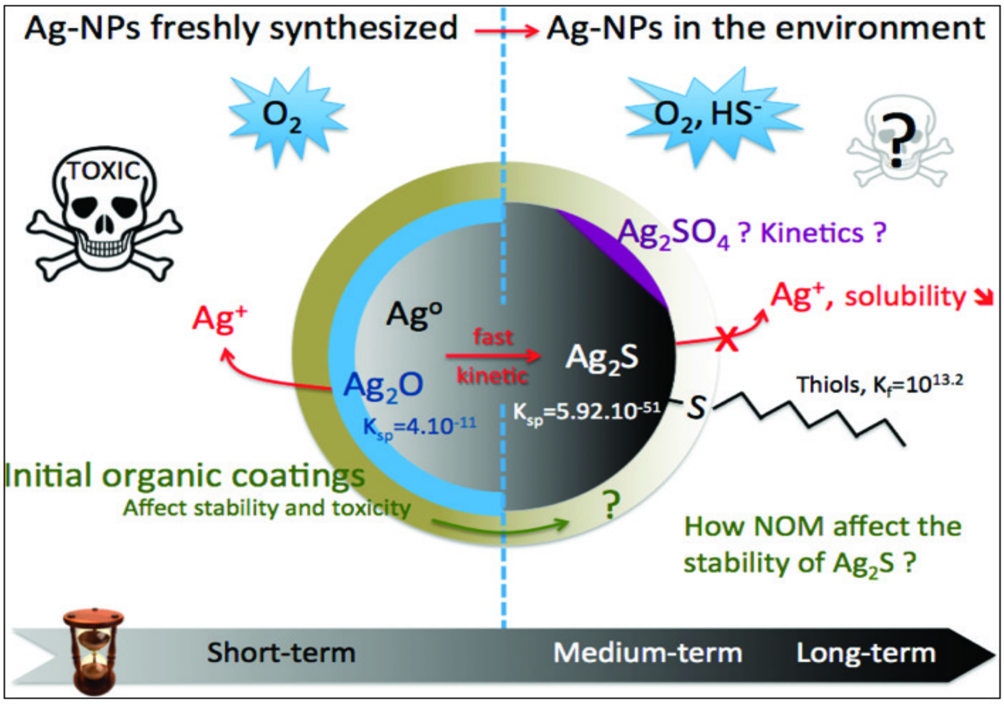

Figure 2: Illustration of the chemical and particle nature of nanomaterials, and the role of the surface properties in determining the transformations that occur, illustrated for the case of Ag nanoparticles. The environmental transformations including coating and surface passivation may reduce the toxicity of the nanomaterials, whereas transformations that lead to enhanced dissolution may increase the toxicity as ionic silver is more toxic generally than particulate nanosilver. From Reidy et al., 2013.

Indeed, regulatory agencies such as the European Chemicals Agency (EChA) have confirmed that nanomaterials are covered under existing chemicals legislation, such as REACH (Registration, Authorisation and Evaluation of Chemicals), although nano-specific provisions have been added as an Annex to the main legislation to address these unique aspects of nanomaterials, and to define nanoforms based on different sizes, surface charges and surface functionalisations (EChA, 2022).

Nanomaterials are characterised by the fact that some of their properties are intrinsic to the composition and unit cell; meanwhile, other properties, mainly those connected to the particle surface, are dependent on their surroundings - these are called extrinsic properties. This means that, when representing nanomaterials it is essential to consider both the core and the surface properties, and when evaluating their toxicity, to consider both the chemical (molecular) and physical (particle-based) impacts. Figure 2 illustrates this for silver (Ag) nanomaterials showing the interplay of bulk and surface chemistries, the reactivity of the surface leading to a range of surface interactions and transformations depending on the range of ligands available in the local environmental surroundings, and the chemical versus physical interactions that can occur.

1.2 Nanomaterials safety assessment

The safety assessment of nanomaterials involves, but is not limited to, the systematic evaluation of potential risks related to their manufacture, usage, and disposal. Key aspects of nanomaterials safety assessment include exposure assessment, hazard identification, and risk characterisation.

1.2.1 Exposure assessment

Understanding how exposure occurs enables identification of potential hazards, implementation of proper safety measures, and minimisation of the potential for adverse effects. There are three primary routes of exposure to nanomaterials, each with its unique set of considerations and potential effects on human health or the environment.

a. Inhalation: Inhalation is a common exposure route for airborne nanomaterials. Workers in industrial settings, where nanomaterials are manufactured or used, are particularly at risk. Inhalation exposure may lead to respiratory issues, systemic toxicity, or even translocation of nanoparticles to other organs.

b. Ingestion: Ingestion of nanomaterials can occur through the consumption of contaminated food or water, or by hand-to-mouth transfer. Ingested nanomaterials may affect the gastrointestinal tract or be absorbed into the bloodstream and transported to other organs.

c. Dermal contact: Skin exposure to nanomaterials can occur in various settings, including occupational exposure, consumer product use, or environmental exposure. Depending on the nanomaterial properties and skin barrier integrity, nanomaterials may penetrate the skin and potentially cause localised or systemic effects.

Assessing the duration and frequency of exposure helps researchers determine the potential cumulative effects of nanomaterials on human health or the environment. Short-term exposure

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may not result in adverse effects, while chronic, repeated exposure could lead to long-term health issues or environmental damage.

Understanding the distribution of nanomaterials in different environmental compartments, such as air, water and soil, is crucial for estimating exposure levels and assessing potential risks. This information helps researchers identify where nanomaterials may accumulate or be transported, which in turn informs risk management strategies and mitigation efforts.

Once the routes of exposure, duration, and frequency of exposure, and the concentrations of nanomaterials in different environmental compartments are known, researchers can estimate exposure levels for different scenarios. This information can be used to identify populations or ecosystems at higher risk of exposure, establish safe exposure limits, and inform the development of safer nanomaterials or alternative applications.

1.2.2 Hazard identification

Hazard identification is a key step in the safety assessment of nanomaterials, and involves evaluating various aspects of nanomaterial toxicity, including cytotoxicity, genotoxicity, immunotoxicity, developmental and neurotoxicity and other potential hazards, to both humans and environmental organisms (Figure 3). To investigate these effects, a combination of experimental methods (of *in vitro* and *in vivo* tests) and computational approaches are applied. Computational approaches, such as quantitative structure-activity relationship (QSAR) modelling and read-across methods, can be used to predict the potential hazards of nanomaterials, by read-across from data-rich materials to related materials for which fewer data exist. These models use existing experimental data to build predictive models, enabling researchers to estimate the toxic effects of untested or novel nanomaterials. Computational methods can complement experimental testing and contribute to the efficient identification of potential hazards, guiding the development of safer nanomaterials and applications.

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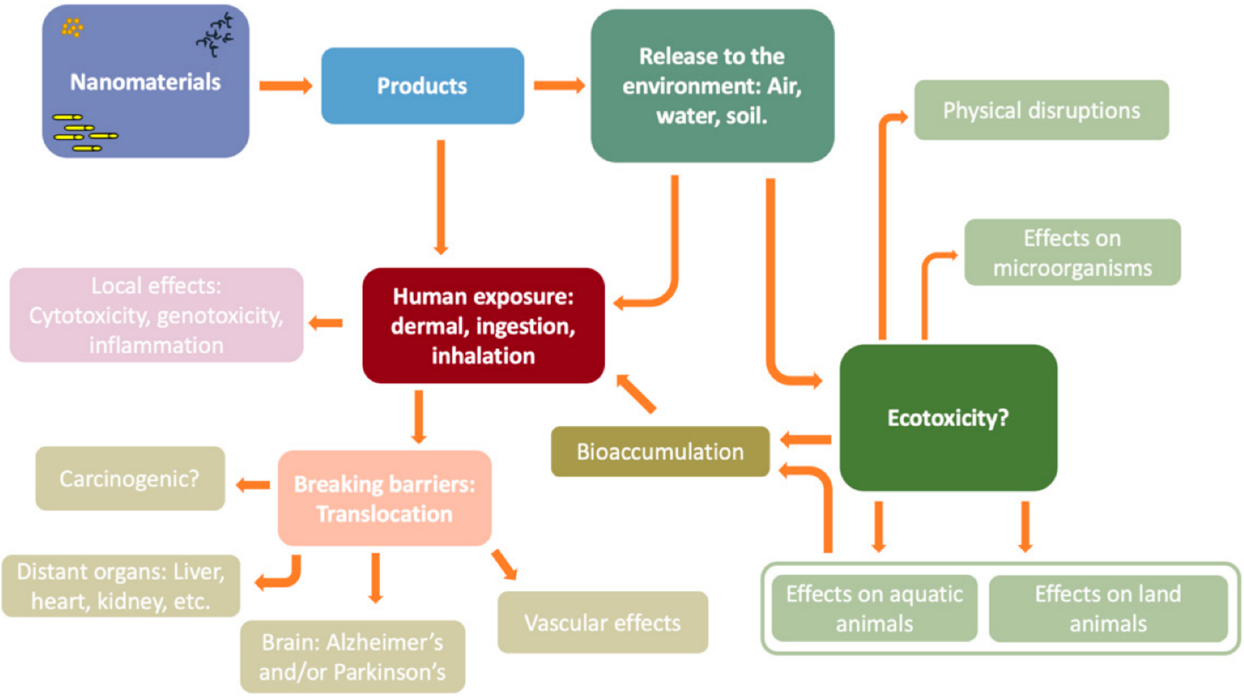

Figure 3: General view of possible interactions, routes of exposure, and adverse outcomes that can be triggered by exposure of humans and the environment to nanomaterials. From Lebre et al., 2022.

1.2.3 Risk characterisation

Risk characterisation integrates information gathered from both exposure assessment and hazard identification to evaluate the potential risks associated with nanomaterials. By synthesising this data, researchers and policymakers can determine whether the risks associated with nanomaterial usage outweigh their potential benefits, ultimately guiding risk management decisions. Key risk management decisions influenced by risk characterisation include setting occupational exposure limits, which are established to protect workers who may come into contact with nanomaterials during manufacturing or handling processes. These limits are designed to minimise potential harm while maintaining a level of exposure deemed safe, based on the available scientific evidence.

1.3 The convergence of nanomaterials and advanced materials: further complexity

As nanotechnology and advanced materials science continue to progress, the convergence of these fields has led to the development of increasingly complex materials with novel properties and applications, presenting new challenges for the assessment and management of risks associated with these innovative materials. Advanced materials, such as biomaterials, smart materials, and self-healing materials, often incorporate nanomaterials to improve their performance or enable

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specific functionalities. This convergence brings additional complexity to the assessment and management of potential risks, including:

Novel properties and behaviours: The interaction between nanomaterials and advanced materials can lead to unique properties and behaviours that are difficult to predict or assess using traditional methods. As a result, researchers need to develop new approaches and tools for characterising these materials and determining their potential impacts on human health and the environment.

Multifunctionality and dynamic properties: The multifunctionality and dynamic properties of these convergent materials make it challenging to assess their safety. For instance, materials that change their properties in response to external stimuli may exhibit different hazards under varying conditions. Understanding the full range of potential hazards requires comprehensive testing and modelling that considers these dynamic properties.

Interdisciplinarity: Assessing the safety of convergent nanomaterials and advanced materials requires a highly interdisciplinary approach, involving collaboration between experts in materials science, nanotechnology, biology, chemistry, engineering, and other fields. This necessitates the development of interdisciplinary research networks and shared resources to foster effective collaboration and information exchange.

New regulatory challenges: The convergence of nanomaterials and advanced materials presents new challenges for regulators, as current regulations may not adequately address the unique properties and potential risks associated with these complex materials. Regulatory frameworks may need to be updated or expanded to ensure the safe development and use of innovative materials.

2. Nanomaterials and nanosafety: defining the domain and the FAIR status prior to WorldFAIR

In early 2022, immediately prior to the start of WorldFAIR, the research infrastructure project NanoCommons[2], in collaboration with the risk governance project Gov4Nano[3], undertook a landscape mapping exercise of FAIR activities underway in NanoSafety cluster projects. This was in order to get an overview on all the major activities from the different EU-funded projects. A detailed questionnaire was developed, and then circulated among all major EU nanosafety projects (via the EU NanoSafety Cluster[4] mailing list of project coordinators). This initiative also reached out to national projects such as the German National Research Data Infrastructure project NFDI4Cat[5], which provided insights into the implementation of the FAIR principles in another domain, partially connected to nanomaterials. In addition, several individual follow-up teleconferences took place, to discuss in detail the FAIR activities of the various projects.

All the input received was firstly merged into a map of FAIR activities, shown in Table 1 which, importantly, points to the many deliverables produced in the respective projects dealing with FAIR data activities and intra-domain considerations. WorldFAIR, which started in June 2022, was not included in this mapping but we have added the relevant information to the table as it is a key part of the ongoing development of FAIR for nanosafety. We note that this table was also presented in NanoCommons Deliverable D9.4, and the data are included in an article that is under review in *Nano Today,* led by the GO FAIR AdvancedNano Implementation Network[6] (Durant et al., 2023).

Table 1: *Summary of the feedback from the questionnaires sent to EU Nanosafety projects forming the landscape map of ongoing FAIR activities in these projects.*

Project	Activities	Since when?	How?	Implementation planned?	Barriers reported
Gov4Nano	WP1 dedicated to FAIR	Since project start	Multiple activities in WP1, eNanoMapper DB, case studies, surveys, GO-FAIR	Ongoing	D1.2

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[2] https://cordis.europa.eu/project/id/731032

[3] https://cordis.europa.eu/project/id/814401

[4] https://www.nanosafetycluster.eu/

[5] https://nfdi4cat.org/en/about-us/

[6] https://www.go-fair.org/implementation-networks/overview/advancednano/

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NanoRIGO	WP7 training events and materials on FAIR data and high quality metadata provision for scientific / technical assessment within nanorisk governance processes	Virtual Venice Nano Training School 2021 and Onsite Venice Nano Training School 2022	Slide sets and recordings from training sessions available online (NSC Youtube channel) based on work driven by Damjana Drobne (Uni Lj) in WP1	ongoing	D7.2
RiskGONE	WP2 Task 2.3	Since project start	eNanoMapper DB, Template Wizard, template harmonisation	Ongoing	
NanoSolveIT	In WP1: Harmonising datasets from supplementary materials of published articles	Since project start	Using semantic web approach (RDF/SPARQL) We have also two efforts for FAIR assessment: 1. General semi-automated FAIR assessment Jupyter notebook (10) 2.Unpublished work on reusability assessment of nanosafety data (FAIR R1.3) using maturity indicators.	Ongoing	
NanoinformaTIX	WP2 Database	Since project start	eNanoMapper DB, Template Wizard, template harmonisation, improvements based on feedback from modellers	Ongoing	
NanoInformaTIX & nanoCommons	Linking omics public data from repositories to eNanoMapper	April 2020	Templates for metadata - Link to repositories	Workflow to systematically process the data	
	Adding persistent identifiers to omics datasets through systematic meta-analysis	Nov. 2020	Data from proteomics repositories is analysed systematically, and descriptors are identified (GO terms, KEGG pathways, etc), which described the results. These descriptors have persistent object identifiers	Starting	

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NanoCommons	several WPs devoted to FAIRification and development of various tools for its promotion	2020	diverse FAIRification initiatives ongoing (FAIRification award, FAIR measures, metadata completeness, SOP development, DMP consulting, etc.	ongoing	D8.3; D9.4; D9.2; Hasenkopf et al. (7)
CHARISMA	WP5 harmonised Raman Database	Since project start	Common format, API, workflows, terminology harmonisation through wikidata	Ongoing	
	Harmonisation of Raman spectroscopy		Standardise Raman protocols	Generate a FAIR Raman data repository	
smartCERIALS	ELN teams based on joint instance map developments for antimicrobial testing strategies	March 2022	data FAIRification initiative for global collaboration between Europe and China	ongoing	
NFDI4Cat	Part of the NFDI initiative to establish modern research data infrastructures for catalysis: - PIDs, - SOPs, - ELNs, - Ontology development, - Training	Oct. 2020	- Creation of a PID for catalysis samples - Establishing (Meta)data standards 4 catalysis - Analysis of requirements for ELNs in catalysis research - New Repository - Ontologies - RDM training	Ongoing	community's insufficient knowledge of FAIR
WorldFAIR	Case studies to advance implementation of FAIR and improve data interoperability / reusability of. Interoperability framework for each case study and research domain. WP4-Nanosafety	June 2022	- Development of a FAIR Implementation (FIP) plan for nanosafety - Development of repository of nano-FAIR training materials - Deployment of approaches for FAIR models / informatics - Implementation of easy-to-use data curation tools	Ongoing	N/A

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2.1 Nanomaterials-specific resources to support FAIR

Here we provide a non-exhaustive snapshot of some of the major resources that are used in the nanomaterials safety community and which currently have different degrees of FAIRness, or are works in progress that are continuously evolving to increase their FAIRNess. Some of the resources listed below were evaluated in 2020 as part of the NanoCommons project, using a semi-automated workflow, to assess their performance against a set of FAIR metrics mapped to the FAIR principles, as described in Ammar et al. (2020).

2.1.1 Databases

The eNanoMapper database[7] provides support for upload, search and retrieval of nanomaterials and experimental data through a REST web services application programming interface (API) and a web browser interface. It is implemented by a customised version of AMBIT web services[8], as described in Jeliazkova et al. (2015). Starting from the chemical compound-centric OpenTox API[9], the eNanoMapper database REST API allows for the representation of chemical substances with complex composition, and experimental data associated with those substances. Nanomaterials are considered a special case of substances, which is consistent with the ontology representations and ECHA guidelines. eNanoMapper is based on a data model originally developed to represent industrial chemicals and implements nanosafety-community-specific solutions aligned with all the FAIR principles, including community-developed standards for regulatory assays and end-points (e.g., Jeliazkova et al., 2016) such as a domain-specific ontology, and generated persistent identifiers (IDs) based on Universally Unique Identifiers. In addition, community-accepted user-friendly IDs are also implemented - for example, nanomaterials IDs assigned by the European Commission's Joint Research Centre (JRC) Nanomaterials Repository[10], and more recently the NanoCommons-developed European Registry of Materials Identifiers (van Rijn et al., 2022). The data model provides a high potential for interoperability through data serialisation into different formats and links to processes and systems for data submission, curation, indexing, federated search, retrieval and analysis workflows. Since 2016, the eNanoMapper data model has been adopted by several European projects, each establishing project-specific eNanoMapper database instances. To provide aggregated findability, accessibility and interoperability across all database instances, the Nanosafety Data Interface[11] was created.

The NanoCommons KnowledgeBase[12] is a web-based resource that provides access to a

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[7] http://data.enanomapper.net/

[8] https://ambit.sourceforge.net/download_ambitrest.html

[9] https://opentox.net/opentox-data-apis

[10] https://joint-research-centre.ec.europa.eu/system/files/2016-06/JRC%2520Nanomaterials%2520Repository-List%2520of%2520Representative%2520Nanomaterials-201606.pdf

[11] https://search.data.enanomapper.net/

[12] https://nanocommons.github.io/user-handbook/data-management/data-resources/NanoCommons-KB/

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comprehensive collection of nanomaterials data and knowledge, and tools to visualise and model the data. The KnowledgeBase includes several features, including:

1. Data Management: The KnowledgeBase provides data upload and download tools and support for curating data related to nanomaterials, including data on their physicochemical properties, toxicity, and environmental impacts.
2. Data Integration: The KnowledgeBase integrates data from various sources and formats, making it easier to discover and access relevant data. Using its semantic mapping approach, synonyms identified and datasets mapped to the underpinning data schema.
3. Ontology-based Annotation: The KnowledgeBase uses an ontology-based approach to annotate and categorise nanomaterials data, making it easier to search and discover relevant information, and supporting the integration of data into the KnowledgeBase.
4. Data Visualisation: The KnowledgeBase provides interactive data visualisation tools for exploring and analysing nanomaterials data, including a dashboard feature summarising the datasets present in the KnowledgeBase.
5. Predictive Modelling: The KnowledgeBase includes tools for predictive modelling of nanomaterials properties and behaviour, such as computational models and machine learning algorithms.

The technical framework of the NanoCommons KnowledgeBase, the BioXM™ Knowledge Management Environment[13], has been described previously (Losko and Heumann, 2017) and consists of a platform-independent Java server–HTML client application. The application backend integrates No-SQL and relational database management and employs a Hibernate layer for object-relation modelling. Therefore, all administrative activities occur on the level of an object-oriented graph model which is automatically transformed into a generic database scheme. Actual information, including ontologies and data, mapped to the object-oriented model form a dense knowledge graph for search, retrieval and analysis. A REST-based web service API provides technical interoperability for transparent tool integration which translates external resources into native reports or analyses delivered by the graphical user interface.

The nanoPharos database[14], developed within the NanoSolveIT and NanoCommons projects, promotes accessibility, interoperability and reusability of curated datasets (from literature or primary data) in a ready-for-modelling format. The nanoPharos database has been designed in line with the FAIR data principles to also include computationally-derived data from simulations of nanomaterials at different levels of complexity. The database was further extended to include nanomaterials characterisation data that can be enriched with a series of atomistic, molecular and structural descriptors, calculated using integrated tools (as for example in Papadiamantis et al.,

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[13] https://www.biomax.com/lib/products/bioxm/Biomax_BioXM_Technical_Profile.pdf
[14] https://db.nanopharos.eu/

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2021). The database offers the possibility of including different batches and instances of the same nanomaterial so as to monitor any physico-chemical transformations across its entire lifecycle.

2.1.2 Ontologies

The eNanoMapper ontology[15] is a standardised terminology that aims to provide a common language for the description and exchange of nanomaterial-related data (Hastings et al., 2015). It was initially developed as part of the eNanoMapper project, and was further extended within the NanoCommons and NanoSolveIT projects, such that it contains over 1,600 classes and 2,500 properties that describe various aspects of nanomaterials, including their physicochemical properties, biological interactions, and toxicological effects. We note that there are some challenges with the acceptance of the eNanoMapper ontology by the community due to lack of terms, mis-matched hierarchy, and mis-defined terms, and as such a harmonisation effort is needed, but it is the most complete nanomaterials ontology currently, integrating as it does the NanoParticle ontology[16] and parts of other relevant ontologies, including the Chemical Entities of Biological Interest (ChEBI)[17] and the Ontology for Biomedical Investigations (OBI)[18] to ensure interoperability and consistency across different domains and data sources. The eNanoMapper ontology is available in the Web Ontology Language (OWL) format.

The Elementary Multiperspective Material Ontology (EMMO)[19] is a formal top-level ontology that provides a comprehensive and multi-perspective representation of materials and their properties. EMMO is designed to provide a unified and structured vocabulary for describing materials and their properties across multiple length and time scales and includes a hierarchical classification of materials, ranging from atoms and molecules to complex materials and devices. EMMO consists of several modules, each representing a different aspect or perspective of materials including their composition, structure, properties, processes, and applications. The ontological framework has been built around concepts like elementary particles, wave-particle dualism, finiteness of space and time intervals coming from the perspective of experimental physics. The development of the middle and upper layers of the ontology has been functional to the respect of these low-level concepts, to facilitate the understanding of the high-level concepts to users with limited or no philosophical background. EMMO was developed using a modular and extensible approach that allows new modules to be added as new perspectives or aspects of materials are identified. It is designed to be interoperable with other ontologies and data formats in the materials domain.

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[15] https://bioportal.bioontology.org/ontologies/ENM
[16] https://bioportal.bioontology.org/ontologies/NPO
[17] https://www.ebi.ac.uk/chebi/aboutChebiForward.do
[18] https://obi-ontology.org/
[19] https://github.com/emmo-repo/EMMO

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2.1.3 Metadata standards (provisional)

ISA-Tab-Nano[20] is the ISA-TAB-Nano extension (Thomas et al., 2013) of the ISA-TAB standard (Investigation/Study/Assay) and was the first attempt to create a structured metadata schema focusing on nanomedicine. It includes the option to semantically annotate the reported data. ISA-TAB-Nano is a complex CSV-type file structure that allows the capture of complex experiments but requires different files to report different types of experiments (e.g., physicochemical characterisation, *in vitro* or *in vivo* assays) and is not designed to account for environmental fate and behaviour studies of dynamic entities such as nanomaterials. Due to its complexity, this is not widely implemented by researchers or nanosafety databases in practice. Simplified versions of the ISA-Tab-Nano approach have been developed via the NANoREG and GRACIOUS projects, among others (Gottardo, et al., 2019).

Another reporting format was defined by the CODATA-VAMAS working group[21] in 2015 (and revised in 2016), the Uniform Description System on the Nanoscale (UDS) (Rumble et al., 2016). UDS focussed on describing the synthesis, physicochemical and structural characterisation of nanomaterials and did not account for complex experiments, their surrounding environment, or the use of computational descriptors and nanoinformatics approaches that are becoming increasingly prominent. ASTM Committee E56 on Nanotechnology has created three Standard Guides or metadata related to the description of nanomaterials (ASTM, 2020).

A recent attempt to develop a data capture template (not a distinct metadata schema), which incorporates the reporting of complex experimental data along with detailed respective metadata, is described by Amos et al., 2021. The Nanomaterials Informatics Knowledge Commons (NIKC) template provides an *Instance Organisational Structure* to map the transformations of nanomaterials in the environment and was developed to capture both the nanomaterials' characteristics and their surrounding environment, while incorporating the different metadata types along with detailed protocols/assays and instruments/consumables used. The NIKC template was modified (simplified and streamlined) via the H2020 NanoCommons infrastructure project[22] (for use initially by the H2020 project NanoFASE to capture complex mesocosm experimental data) and has since been expanded to cover complex biomolecule corona interactions with nanomaterials (Martinez et al., 2020) and even nanomaterials-containing mixture datasets (Martinez et al., 2023). The Instance Organisational Structure captures the transformational journey of a nanomaterial by sorting the experimental data into five categories: instance, material, medium, property, and supplementary. Each of the five categories catalogue the metadata describing the nanomaterial and the exposed organism, noting where the nanomaterials characteristics might be transformed, e.g., by biomolecule binding, uptake or other transformation.

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[20] https://wiki.nci.nih.gov/display/ICR/ISA-TAB-Nano
[21] https://codata.org/initiatives/previous-codata-working-groups/nanomaterials/
[22] https://www.nanocommons.eu/overview/

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Building on the Instance Organisational Structure concept, Instance Maps[23] provide a visual representation of the relationships between different elements of an experiment or study, including materials, experimental conditions, and observed properties. These maps can help researchers better understand the complex interactions and transformations that occur during nanosafety experiments, making it easier to interpret and analyse the data. Instance Maps offer a powerful tool for organising, visualising, and analysing complex data in nanosafety research. Key benefits of Instance Maps include:

- Comprehensive data representation: Instance Maps visually represent the relationships between various elements of an experiment or study, such as materials, experimental conditions, and observed properties. This comprehensive view allows researchers to better understand complex interactions and transformations that occur during nanosafety experiments, aiding in data interpretation and analysis.
- Detection of data gaps: Instance Maps can help researchers identify missing or incomplete data in their experiments, highlighting areas that require further investigation or clarification. This allows for a more thorough understanding of nanomaterial safety and supports the development of more comprehensive risk assessments.
- Facilitated data integration and comparison: Instance Maps provide a standardised format for representing complex experimental data, simplifying the comparison of results across different studies. This standardisation enables more effective data integration and analysis, leading to more robust insights and conclusions.
- Improved reproducibility: By offering a clear visual representation of experimental conditions and results, Instance Maps contribute to better reproducibility in nanosafety experiments. This ensures that results are reliable, accurate, and can be replicated by other researchers.
- Accelerated discovery and innovation: Instance Maps facilitate a deeper understanding of nanomaterial behaviour and safety by improving data organisation, visualisation, interoperability, and collaboration. As a result, researchers can more rapidly gain new insights, informing the design of safer nanomaterials and promoting responsible risk management strategies.

Integrating Instance Maps into metadata standards and tools promotes adherence to FAIR principles: Instance Maps improve the findability of experimental data by organising and visually representing complex relationships, making it easier for researchers to locate relevant information. By providing a standardised format for data representation, Instance Maps enhance accessibility and enable seamless sharing of data among researchers. Additionally, Instance Maps facilitate interoperability by adopting a consistent structure for organising and connecting data points, allowing for more effective integration and comparison of data from different studies. Finally,

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[23] https://nanocommons.github.io/user-handbook/data-management/instance-maps/

instance maps can support reusability by offering a clear and intuitive representation of experimental conditions and results, which can be easily understood and replicated by other researchers. Incorporating Instance Maps into metadata standards and tools will support effective management of experimental metadata and data.

The Template Wizard[24], developed within the RIskGONE project and now extended more widely, is a web-based tool that enables researchers to create and share (meta)data templates for nanosafety experiments. The Template Wizard is a web form, where the user can enter metadata of the experiment and download a customised data entry template. There are different templates for physico-chemical properties, ecotoxicology, *in vitro* hazard assessment, and exposure and release experiments, and if a template is not available yet for a specific endpoint, the workflow to create the required template from the existing templates is documented.

With the Template Wizard, users can create templates that define the structure and content of experimental data for a particular type of nanosafety experiment. The tool provides a user-friendly interface for defining the structure of the template, including the data fields and metadata that should be included. Users can also specify controlled vocabularies and ontologies to ensure consistency and interoperability of the data. Once the template has been defined, it can be exported in a variety of formats including JSON, RDF, and CSV. The template can also be shared with other researchers, either by providing a download link or by publishing the template to the library of templates. The tool also enables researchers to easily share and compare data across experiments, which can facilitate the development of more accurate and predictive models of nanomaterial behaviour and toxicity.

2.1.4 Identifiers

The management of nanomaterials and nanosafety data calls for adherence to the FAIR principles. Ensuring the FAIR management of data requires the creation of unique, global identifiers for each type/family/batch of nanomaterials. Existing synthesis processes result in significant heterogeneity of particle properties within and between batches, and as such, nanomaterials are best considered as ensembles or collections of entities, as described in the CODATA Universal Description System (Rumble et al., 2016) and shown schematically in Figure 4.

The Universal Description System for nanomaterials divides nanomaterials and the objects that contain them into four major types, which each type of nanomaterial requiring slightly different sets of information to describe it completely:

- An individual nano-object (i.e. a single particle)
- A collection of nano-objects, described as per Figure 4 which can be:

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[24] https://search.data.enanomapper.net/datatemplate/default/

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  - Identical nano-objects
  - Different nano-objects
- A bulk material containing individually identifiable nano-objects
- A bulk material that has nano-scale features.

A collection of nano-objects is defined as a group of two or more nano-objects, and the nano-objects within the collection can be associated in a variety of ways, including direct bonding, van der Waals attraction, electrostatic interactions, or third party mediation (e.g., catalyst).

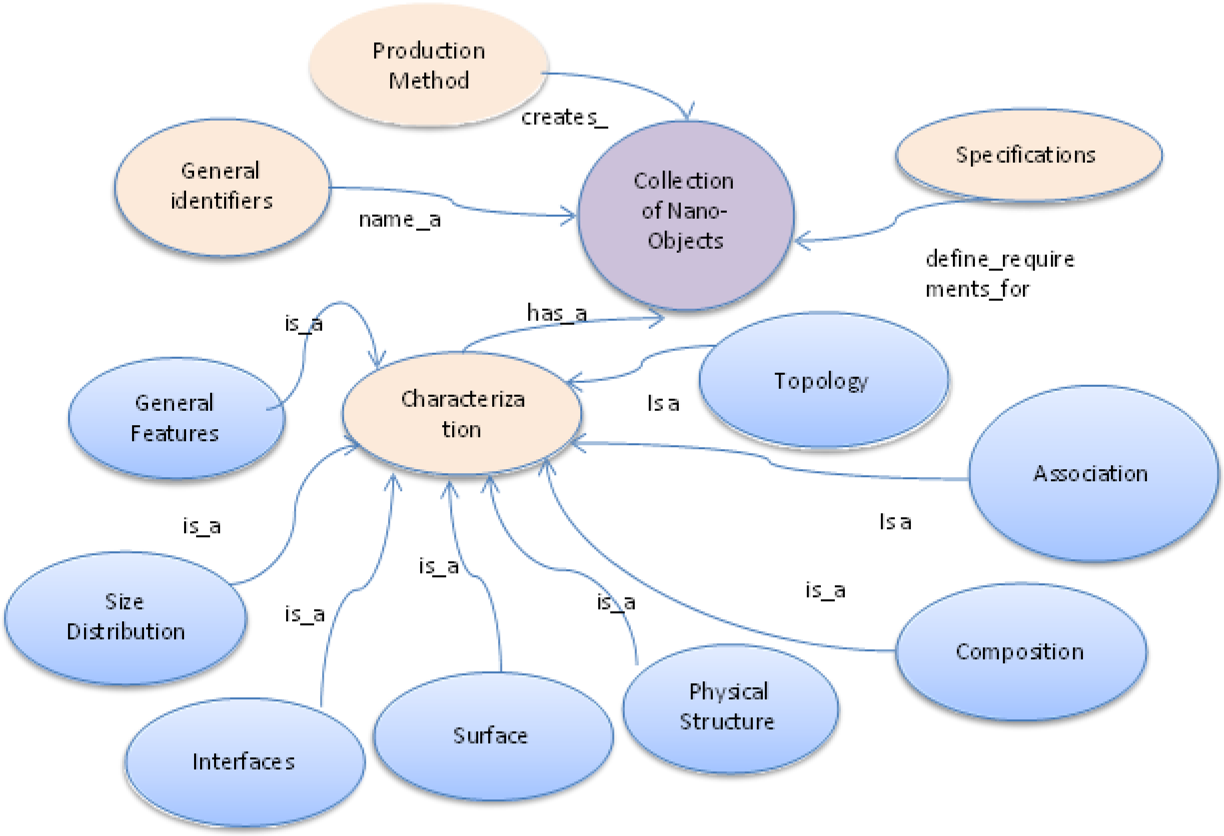

Figure 4. Schematic of the information categories needed to describe a collection of nano-objects.

Given the three-dimensional nature of nanomaterials, and their existence as collections of nano-objects, existing identifiers may not always be suitable for representation of the specific nanomaterials used in a particular project and its studies, leading to the use of textual descriptions in research project communications and reporting. To address this issue, the European Registry of

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Materials (ERM) Identifier and Nanomaterials InChI have been introduced as new identifiers (van Rijn et al., 2022; Lynch et al., 2020).

The European Registry of Materials[25] (ERM) supports the FAIR management of nanomaterials, providing identifiers that serve as part of the metadata, indicating that different documents and datasets relate to the same material (van Rijn et al., 2022). The ERM doesn't define or provide knowledge about a specific material, but it functions as a unique global identifier linking all information and metadata, thereby ensuring the FAIR dissemination of knowledge about that material. Assigning an ERM identifier before experiments begin allows projects to manage their internal data, aiming to make data open and FAIR in the long term. The ERM allows for the consistent identification of materials by multiple partners within the same project. The full value of ERM identifiers will become clear when more research outputs are publicly shared, allowing for accurate connections between results.

Chemoinformatics has developed efficient ways of representing chemical structures for small molecules as simple text strings, such as Simplified Molecular-Input Line-Entry System (SMILES) and the IUPAC International Chemical Identifier (InChI), which are machine-readable. The next frontier is encoding the multi-component structures of nanomaterials (NMs) in a machine-readable format to enable linking of datasets for nanoinformatics and regulatory applications. The H2020 research infrastructure NanoCommons and the nanoinformatics project NanoSolveIT have analyzed issues involved in developing an InChI for NMs (NInChI), as described in Lynch et al., 2020.

The NInChI system for nanomaterials is designed to comprehensively capture the complex structures of these materials by incorporating multiple layers of information. These layers include the core composition, which may be multi-layered, surface topography, surface coatings or functionalisation, doping with other chemicals, and the representation of impurities. Additionally, the system takes into account nanomaterial distributions, the types of chemical linkages connecting surface functionalisation and coating molecules to the core, and the various crystallographic forms exhibited by nanomaterials. This multi-layered approach ensures that the NInChI system provides a thorough and accurate representation of nanomaterial structures, facilitating improved data exchange and collaboration in the field. The development of a computer-readable code that uniquely specifies a nanomaterial while recognizing the inherent complexity of nano-objects is crucial for the progress of nanoinformatics. This allows for standardisation in naming conventions, facilitating harmonised database searching for regulatory registration, grouping, classification, and modelling of nanomaterials.

The InChI Working Group on Nanomaterials[26] and the CODATA Task Group on extension of the InChI to nanomaterials[27] are collaborative efforts aimed at developing a standardised and

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[25] https://github.com/NanoCommons/identifiers/tree/2022-03

[26] https://www.inchi-trust.org/inchi-working-groups/#nano

[27] https://codata.org/initiatives/task-groups/extension-of-inchi-for-nanomaterials/

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machine-readable naming convention for nanomaterials. The InChI Working Group focuses on encoding information about nanomaterials' composition, size, shape, and surface chemistry into an extended version of the IUPAC International Chemical Identifier, known as NInChI. This group aims to leverage best practices from other InChI working groups, such as those for mixtures, reactions, and polymers. Meanwhile, the CODATA Task Group on extension of the InChI to nanomaterials builds upon the Uniform Description System (UDS) for materials at the nanoscale and collaborates with the NInChI Working Group to develop test cases, based on the metadata defined within the UDS. The Task Group is curating extensive datasets of commercial nanomaterial structures, conducts hackathons with experts, and works on the implementation and evaluation of the NInChI system. Their goal is to provide a fully-documented and tested extension of the InChI for nanomaterials, with guidelines and training materials for its adoption submitted to IUPAC by mid-2023 and updating of the existing demonstrator tool[28] to encode the revised NInChI standard.

In the case of the Nanomaterials InChI we focus on the *collection of nano-objects* as defined in the Universal Description System, and shown in Figure 4 above, which can be either identical (consider the case of highly monodisperse, highly pure nanomaterials such as gold (Au) nanomaterials whose size can be very tightly controlled) or different nano-objects reflecting the aforementioned polydispersity in physicochemical properties contained in a typical batch of nanomaterials.

The development and implementation of the Extension of InChI for Nanomaterials (NInChI) aligns with the WorldFAIR project and FAIR data principles. By enabling a standardised and machine-readable identification and representation system for nanomaterials, NInChI will help to promote Findability, Accessibility, Interoperability, and Reusability of data associated with nanomaterials. Implementation studies are being used to understand efficacy and best practices for inclusion into data models.

Findability: The NInChI system is intended to ensure that nanomaterial data is easily discoverable, as each nanomaterial receives a unique identifier, improving the ability to search and find specific materials and their associated data across multiple platforms, databases, and research publications.

Accessibility: NInChI will contribute to the accessibility of data by providing a standardised naming convention and structure that allows researchers, regulators, and industry professionals to easily access, understand, and work with data related to specific nanomaterials. The test implementations currently being developed will be used to demonstrate how NInChI facilitates harmonisation of database search mechanisms for grouping, classification, and modelling of nanomaterials.

Interoperability: The NInChI system enhances the interoperability of nanomaterial data, enabling seamless exchange and integration of information between different databases, systems, and research groups. The machine-readable format of NInChI ensures that data can be easily shared, compared, and combined, leading to better collaboration and synthesis of findings.

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[28] http://www.enaloscloud.novamechanics.com/nanocommons/NInChI/

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Reusability: With a standardised naming convention and clear guidelines for usage, NInChI promotes the reusability of nanomaterial data. Providing curated and well-documented nanomaterial descriptions, associated characterization data, and in due course NInChIs, will ensure that nanomaterials data can be easily reused and repurposed for future research and applications, leading to increased efficiency and reduced redundancy in data generation.

It is worth noting that none of these are fully implemented community standards as yet, as further work is needed in all cases (Papadiamantis et al., 2020), but they provide a strong basis from which to formalise the required community-agreed metadata standards for nanomaterials.

3. FAIR Implementation Profiles

Broadly speaking, the FAIR Principles (Wilkinson et al., 2016) can be partitioned into two groups: those that address the technological solutions and infrastructure needed to be FAIR and those that address the data content and as such are domain-specific. For simplicity we refer to the FAIR Principles focusing on IT and infrastructure as the Red principles, and those on the domain-relevant content as the Blue principles (Figure 5) as described in Schultes, 2023. The Red principles focus on the capabilities of the data infrastructures and are mostly agnostic to the actual content and specialised domain requirements. Conversely, the Blue principles represent implementation choices that must be made by practising domain experts (e.g., the research scientists, project consortia), and include standards and technologies around metadata formats and domain-specific ontologies, vocabularies and semantics.

A FAIR (Findable, Accessible, Interoperable, Reusable) Implementation Profile is a set of guidelines and recommendations that provide a standardised approach for ensuring that data and digital resources are compliant with the FAIR principles. A FAIR Implementation Profile (FIP) is a list of declared technology choices (including which standardised metadata the community use, which persistent identifiers are applied to the data, and which machine-readable formats are utilised to enable searching of the datasets), also referred to as FAIR Enabling Resources (FERs) – see Table 2 for a glossary of some key terms related to FIPs, that are intended to implement one or more of the FAIR Guiding Principles, made as a collective decision by the members of a particular community of practice.

A FIP thus specifies the technical and organisational requirements necessary for making data and digital resources FAIR.

A FIP can be compiled to declare the current status of implementations within a community (called the ‘As-Is’ FIP). This declaration can also sometimes be useful in guiding data stewards working in that community.

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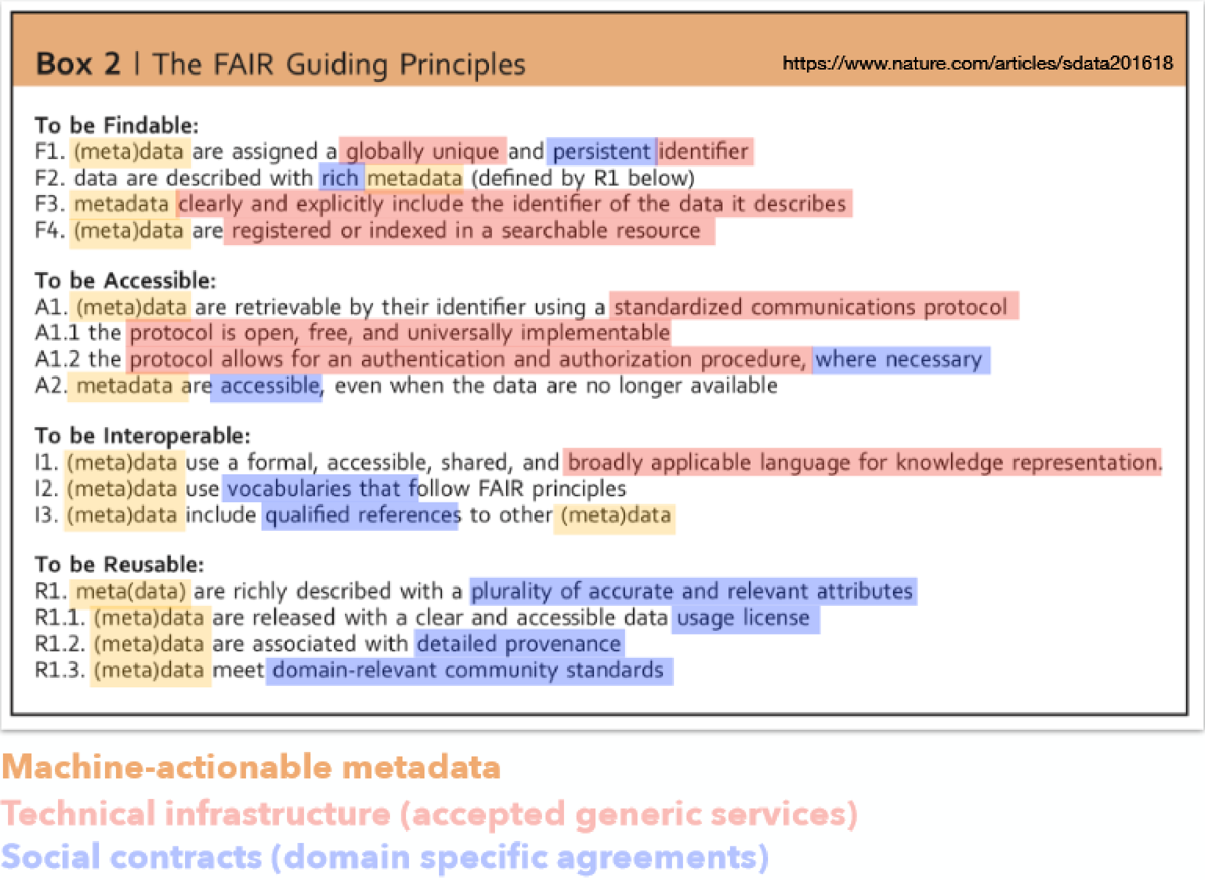

Box 2 | The FAIR Guiding Principles https://www.nature.com/articles/sdata201618

To be Findable:
F1. (meta)data are assigned a globally unique and persistent identifier
F2. data are described with rich metadata (defined by R1 below)
F3. metadata clearly and explicitly include the identifier of the data it describes
F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:
A1. (meta)data are retrievable by their identifier using a standardized communications protocol
A1.1 the protocol is open, free, and universally implementable
A1.2 the protocol allows for an authentication and authorization procedure, where necessary
A2. metadata are accessible, even when the data are no longer available

To be Interoperable:
I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
I2. (meta)data use vocabularies that follow FAIR principles
I3. (meta)data include qualified references to other (meta)data

To be Reusable:
R1. meta(data) are richly described with a plurality of accurate and relevant attributes
R1.1. (meta)data are released with a clear and accessible data usage license
R1.2. (meta)data are associated with detailed provenance
R1.3. (meta)data meet domain-relevant community standards

Machine-actionable metadata
Technical infrastructure (accepted generic services)
Social contracts (domain specific agreements)

Figure 5: The FAIR Guiding Principles, as originally published in 2016, are partitioned into those associated primarily with technical implementation (highlighted in red) and those associated with content-related, domain-relevant standards and practices (highlighted in blue). Yellow highlights the pervasive role of metadata throughout the FAIR Principles. From Schultes, 2023.

Alternatively, a FIP can be compiled to decide on the future use of FERs in a community (called the ‘To-Be’ FIP). These FIPs can be used to document technology trends in FAIR.

It is likely that FIPs will need periodic revision. Each new version documents improvements in FAIR over time.

Any given FIP can be compared with FIPs from other communities giving insight on how FIPs might be optimised to ensure FAIR Convergence.

Table 2: Glossary of terms related to FAIR Enabling Resource types as used in the development of the WorldFAIR Nanomaterials As-Is FIP

Term	**Definition**	**Link to ontology term**
FAIR Enabling Resource	A FAIR Enabling Resource is a digital object that provides functions needed to achieve some aspect of FAIRness addressessing explicitly one FAIR Sub-Principle.	https://w3id.org/fair/fip/terms/FAIR-Enabling-Resource
FAIR Supporting Resource	FAIR Supporting Resource (FSR) is any resource that supports the FAIRification or FAIR Orchestration of data and metadata. FSRs are identified with a GUPRI and have a machine-readable representation as a nanopublication which includes metadata about it. There are different types of FSRs.[29]	Currently being implemented into the ontology
metadata schema	A specification (schema) that specifies metadata fields describing attributes of data or other digital objects.	https://w3id.org/fair/fip/latest/Metadata-schema
identifier service	An identifier Service provides for any digital object (1) algorithms guaranteeing global uniqueness, (2) policy document	https://w3id.org/fair/fip/latest/Identifier-service

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[29] Definition from https://fairconnect.pro/fair-supporting-resources

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Term	Definition	Link to ontology term
	that guarantees persistent and (3) resolution of the identifier to machine-actionable metadata describing the object and its location (FAIR Principle F1).	
metadata-data linking schema	A Metadata-Data Linking Schema is a specification (schema) that provides a unique, persistent, (ideally) bi-directional, machine-actionable link between metadata and the data they describe (F3).	https://w3id.org/fair/fip/latest/Metadata-data-linking-schema
registry	A Registry is a service that indexes metadata and data and provides search over that index (F4).	https://w3id.org/fair/fip/terms/Registry
communication protocol	A Communication Protocol is a specification of how messages are structured and exchanged (A1.1).	https://w3id.org/fair/fip/latest/Communication-protocol
authentication and authorisation service	An Authentication and Authorisation Service is a service that mediates access to digital objects according to specified conditions (A1.2).	https://w3id.org/fair/fip/latest/Authentication-and-authorization-service
metadata preservation policy	A Metadata Preservation Policy is a document that describes the conditions under which metadata are to be provisioned in the future (maybe part of a data management plan) (A2).	https://w3id.org/fair/fip/latest/Metadata-preservation-policy
knowledge representation language	A Knowledge Representation Language is a language specification whereby knowledge can be made processible by machines (I1).	https://w3id.org/fair/fip/latest/Knowledge-representation-language

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Term	Definition	Link to ontology term
structured vocabulary	A Structured Vocabulary is a controlled list of uniquely identified and unambiguous concepts with their definitions represented preferably using web standards (I2).	https://w3id.org/fair/fip/latest/Structured-vocabulary
semantic model	A Semantic Model is a specification that defines qualified relations between entities describing data or other digital objects using structured vocabularies (I3).	https://w3id.org/fair/fip/latest/Semantic-model
data usage licence	A Data Usage Licence is a document that describes the conditions under which a digital object can be legally used (R1.1).	https://w3id.org/fair/fip/terms/Data-usage-license
provenance model	A Provenance Model is a specification (schema) that specifies metadata fields describing the origin and lineage of data or other digital objects (R1.2).	https://w3id.org/fair/fip/latest/Provenance-model

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3.1 The FIP Wizard

The FIP Wizard[30] is a web-based tool developed by the FAIRsFAIR project that helps organisations create FIPs for their data and digital resources. The FIP Wizard provides a structured approach for creating and implementing a FIP, guiding users through a step-by-step process for creating a FIP, starting with selecting a domain or discipline for the FIP. The tool provides a template for each of the sub-principles of the four FAIR principles (findability, accessibility, interoperability, and reusability), with existing FAIR-Enabling Resources (FERs) being searchable, and FERs that have been approved by the GO FAIR Foundation identified with a GFF symbol. Users can select FERs based on their community practice or to fit their specific needs, and can also add additional fields or FERs as needed, which are then minted as nanopublications.

Once the FIP is created, the FIP Wizard provides guidance on how to implement the FIP, including how to evaluate existing digital resources for their FAIRness and how to develop a roadmap for achieving FAIRness over time. The tool also provides resources and links to further information on FAIR principles and best practices.

The guidelines for preparing a FIP[31] provide a practical 'how to' overview for researchers and data stewards who wish to create a FIP using the FIP Wizard 3.0 tool. The use of nanopublications, an RDF-based format to represent scientific data (Kuhn et al., 2015), and the FIP Ontology[32] enables FIPs themselves to be FAIR: the FIP Wizard 3.0 uses (consume and produce) nanopublications which allows the various elements of the FIP to be captured in a highly modular, referenceable, machine-readable format.

General background on the FIP and its role in driving convergence is provided in Schultes et al. (2020) which introduces the FAIR hourglass and other concepts.

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[30] https://fip-wizard.ds-wizard.org/
[31] https://osf.io/5ygzx
[32] https://peta-pico.github.io/FAIR-nanopubs/fip/index-en.html

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3.2 The WorldFAIR Nanomaterials Case Study (WP04) as described in D2.1

Leads and partners: University of Birmingham (UK), 7past9 (Germany), NovaMechanics (Cyprus); partners in a number of nanomaterials and nanosafety activities, including NanoCommons, and the CODATA Task Group on NanoInChI.

Focus of Case Study: This Case Study will enable the further adoption of the FAIR principles by the international nanomaterials community and encourage greater alignment with neighbouring disciplines and communities. It builds on the partners' successful collaboration in NanoCommons (a research infrastructure for nanoinformatics and FAIR nanomaterials data) and their leadership of the IUPAC efforts to develop a standard extension of the InChI for nanomaterials.

Focus of the WorldFAIR Nanomaterials As-Is FIP: The NanoCommons community infrastructure (serving the European Nanotechnology Data, Knowledge and Informatics Community and started by the NanoCommons infrastructure project) is intended to be the data and knowledge hub of the EU NanoSafety Cluster coordinating nanosafety research in Europe. Led by three core partners (UoB, 7P9 and NovaM, who were also partners in the NanoCommons project), the community infrastructure connects all stakeholders from current nanomaterials and new advanced materials projects to foster knowledge exchange and harmonisation of the data ecosystem.

3.2.1 Declaring the WorldFAIR Nanomaterials community

A first step in establishing a FIP is to define the community to whom the FIP is applicable. In this case, for the initial 'As-Is' FIP for nanomaterials safety, we defined the community as being: *The Nanosafety Community involved in NanoCommons / FAIR activities and the GO FAIR AdvancedNano Implementation network.*

This was further refined to be:
European Nanotechnology Data, Knowledge and Informatics Community. Started by the NanoCommons infrastructure project, the NanoCommons community infrastructure is intended to be the data and knowledge hub of the EU NanoSafety Cluster coordinating nanosafety research in Europe. Led by three core partners from the NanoCommons project and now in the WorldFAIR project, it is connecting all stakeholders from current nanomaterials and new advanced materials projects to foster knowledge exchange and harmonisation of the FAIR nanosafety data ecosystem.

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3.2.2 The Initial WorldFAIR As-Is Nanomaterials FIP (as downloaded from the FIP Wizard)

Publication Date	2023-05-10T00:29:23.722503351Z
Community	European Nanotechnology Data, Knowledge and Informatics Community (NanoCommons, AdvancedNano IN and WorldFAIR)
Data Steward	0000-0003-4250-4584
Start Date	2022-10-01
End Date	2024-05-31

	FAIR Enable Resource (FER)			**Replacement FER**		
Question	**Name**	**URI**	**Usage**	**Name**	**URI**	**Considerations**
F1 MD	DOI | Digital Object Identifier	http://purl.org/np/RAnAWGdeI_1GGmDAqv-vZjby5XqbL2ZujNz1vgwK_6cRI#DOI	currently in use			Unique identifiers for datasets
F1 MD	ORCID | Open Researcher and Contributor ID	http://purl.org/np/RA1MzU1MPio-mtLzm1P7zfTBSMnTNc2I8HLNARhPjpif8#ORCID	planned use			Unique identification of data providers.

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F1 MD	International Standard Name Identifier for an identity.	http://purl.org/np/RAcz7lapLgpze_yMNsg47W08YokhONacTYbWhm-Foyda0#ISNI	planned use			Unique identification of provider's institution.
F1 MD	UUID | Universally Unique Identifier	http://purl.org/np/RA5ikgqnKqn071dwzXFdiXlnM8hWZRdFKsQjC_e5YRkEw#UUID	currently in use			eNanoMapper DB and project-specific DBs based on eNanoMapper (NANoREG, Nanoreg2,...)
F1 MD	URI | Uniform Resource Identifier	http://purl.org/np/RA5-OsT0-sjRbcoFEGfOzkrcFtExipMRmoLErzg5QWL7c#URI	currently in use			OpenTox API
F1 MD	ROR | Research Organization Registry	http://purl.org/np/RAFP-uWPTN5u2kPR8pYelgdbwyP1_KYZgoogYlv0Wp-fQ#ROR	currently in use			Unique identification of provider's institution promoted by RDA.
F1 D	DOI | Digital Object Identifier	http://purl.org/np/RAnAWGdeI_1GGmDAqv-vZjby5XqbL2ZujNz1vgwK_6cRI#DOI	currently in use			The community would like to establish a mechanism to cite data(sets) in scientific publication to better show the value of data and increase the incentive to make it publicly available. DOIs, often in addition to data warehouse specific unique identifiers, will help with that since they put the datasets on the same level as other citations.
F1 D	URI | Uniform Resource Identifier	http://purl.org/np/RA5-OsT0-sjRbcoFEGfOzkrcFtExipMRmoLErzg5QWL7c#URI	currently in use			Database specific identifiers

F2	DataCite Metadata Scheme	http://purl.org/np/RAko0U2Q8boW-drM8t11DcbX6Ixu2mcSQf-2BrM07geIQ#datacite_metadata_scheme	currently in use			Used to get the DOIs
F2	Schema.org Dataset	http://purl.org/np/RAfpqImxNsTJLDAV3ZvcQBOddyZf-Yhl2WHXFpGHOLe-Y#Schema.org_Dataset	currently in use			Currently mainly used to annotate websites with training contents. Schema.org and bioschemas.org are proposed to be used more widely.
F2	DC | Dublin Core	http://purl.org/np/RApwFvegOdPfNuKlF64wctAzaffAv3j_2kAU9y6kfBoy8#DCMI	planned use			Implementation was tested in the prototype combining institutional repositories and nano-specific warehouses.
F2	Frictionless datapackage metadata standard	http://purl.org/np/RA3ANxquLS74NljEgj7Z9zGzEwwZRv8cc8BcCX1YjlFkY#Frictionless	planned use			Implementation was tested in the prototype combining institutional repositories and nano-specific warehouses.
F4 MD	Zenodo	http://purl.org/np/RAQKRYjUrndhJAbsgnuhr1Z3DecqtWVl1qUTC2cPpyLDY#Zenodo	currently in use			Possibility to get DOI for (meta)data
F4 MD	NanoCommons Knowledge Base	http://purl.org/np/RA1kA_6seb_Ea7QzQjZjSvZjfoEJf8r-78Zpz4_PE7Nng#NanoCommons	currently in use			Indexing of data from the NanoCommons data warehouse and other nano-specific databases implemented as part of the NanoCommons project.

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F4 MD	Google Dataset Search	http://purl.org/np/RAUhotKhSj2m1ftHGPXAYyL2QgY60L6mYrunOzQwGZJ44#Google_Dataset_Search	to be replaced	NanoCommons Knowledge Base	http://purl.org/np/RA1kA_6seb_Ea7QzQjZjSvZjfoEJf8r-78Zpz4_PE7Nng#NanoCommons	Promoted as one way to make data better findable. However, this leads to data duplication which should be avoided by the generally agreed nano-specific solution integrated into the European data ecosystem.
F4 MD	NSC open dataset inventory	http://purl.org/np/RAjovVPhMA4bCa0SVhPre5x17hn1mPqc5rjtPpRoSh-uM#NSCOpenData	currently in use			Similar to institutional repositories, this listing needs to be integrated into (or even replaced by) a more general solution. Even if this might be helpful for getting datasets provided e.g., as supporting material of scientific publications into this general solution, the need to curate the metadata manually limits the available entries.
F4 D	Google Dataset Search	http://purl.org/np/RAUhotKhSj2m1ftHGPXAYyL2QgY60L6mYrunOzQwGZJ44#Google_Dataset_Search	to be replaced	NanoCommons Knowledge Base	http://purl.org/np/RA1kA_6seb_Ea7QzQjZjSvZjfoEJf8r-78Zpz4_PE7Nng#NanoCommons	Promoted as one way to make data better findable. However, this leads to data duplication which should be avoided by the generally agreed nano-specific solution integrated into the European data ecosystem.
F4 D	NanoCommons Knowledge Base	http://purl.org/np/RA1kA_6seb_Ea7QzQjZjSvZjfoEJf8r-78Zpz4_PE7Nng#NanoCommons	currently in use			Database provided by the NanoCommons project to host data from many different EU funded projects.

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F4 D	eNanoMapper database	http://purl.org/np/RATFtaElhlwVkGRPb0PBDiSh1NnZ-yUBKiROaGZ2F796M#eNM	currently in use			Database provided by the eNanoMapper project to host data from many different EU funded projects.
F4 D	nanoPharos database	http://purl.org/np/RAV8n1_dl6yXvoryYdX9nUwk_Ym0jiVWgFhikw3STq3b4#nanoPharos	currently in use			Database specifically designed to provide data for model development and nanoinformatics applications
A1.1 MD	REST | Representational state transfer	http://purl.org/np/RAszH6lU-Zc3UO7MHPKj1Lb0dmMmaTJrRvQ0jqpXMyFY4#REST	currently in use			Work on harmonisation of REST APIs provided by data warehouses and modelling tools was done in eNanoMapper, OpenRiskNet and NanoCommons / some SOAP APIs are also available / data access from many databases as HTML
A1.1 D	FTP | File Transfer Protocol	http://purl.org/np/RARv4EFw3iwjRn01xnpto4yzc15buTVcm2_q-8a3jLoZw#FTP	currently in use			Mainly used for omics and MS data to upload and access data from standards (not-nano-specific) databases.
A1.1 D	REST | Representational state transfer	http://purl.org/np/RAszH6lU-Zc3UO7MHPKj1Lb0dmMmaTJrRvQ0jqpXMyFY4#REST	currently in use			Work on harmonisation of REST APIs provided by data warehouses and modelling tools was done in eNanoMapper, OpenRiskNet and NanoCommons / some SOAP APIs are also available / data access from many databases as HTML

A1.2 MD	OAuth | Open Authorization	http://purl.org/np/RAbhClJzwMFVkgwvrhsdjnpxtH58oLKoyxgj60DzkS-q4#OAuth	currently in use			To my knowledge is this the underlying mechanism of the EOSC and ELIXIR A&A
A1.2 MD	Keycloak Single-Sign On	http://purl.org/np/RAOhpi4pd0_dAOReqbH_p9URwV30ErkyGK775n4lb9VJg#Keycloak	currently in use			Used in the OpenRiskNet project, which was partly based on Red Hat sponsored services.
A1.2 D	OAuth | Open Authorization	http://purl.org/np/RAbhClJzwMFVkgwvrhsdjnpxtH58oLKoyxgj60DzkS-q4#OAuth	currently in use			Data and metadata are accessed using the same A&A mechanisms.
A1.2 D	Keycloak Single-Sign On	http://purl.org/np/RAOhpi4pd0_dAOReqbH_p9URwV30ErkyGK775n4lb9VJg#Keycloak	currently in use			Data and metadata are accessed using the same A&A mechanisms.
I1 MD	OWL | Web Ontology Language	http://purl.org/np/RAIpnldLlIedp5J7Jcy8pt_X9_YpOez4rO-fHxZl0T96Y#OWL	currently in use			Used to represent the eNanoMapper ontology.
I1 MD	RDF | Resource Description Framework	http://purl.org/np/RAutRQwoS4d5eLq7eBV1xsnWZ2spDYH4xfhhRzOxSZdhs#RDF	currently in use			Different RDF data source exist.
I1 MD	JSON-LD | JavaScript Object Notation for Linking Data	http://purl.org/np/RAQKjgd7Ug9xSo4J0REW_AHGOJyaF9-ydj60nunqQ0qVg#JSON-LD	currently in use			JSON-LD is used to annotate API results in different modelling tools (started in OpenRiskNet)
I1 D	JSON-LD | JavaScript Object Notation for Linking Data	http://purl.org/np/RAQKjgd7Ug9xSo4J0REW_AHGOJyaF9-ydj60nunqQ0qVg#JSON-LD	currently in use			See Declaration I1a.

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I1 D	RDF | Resource Description Framework	http://purl.org/np/RAutRQwoS4d5eLq7eBV1xsnWZ2spDYH4xfhhRzOxSZdhs#RDF	currently in use			See Declaration I1a.
I1 D	OWL | Web Ontology Language	http://purl.org/np/RAIpnldLlIedp5J7Jcy8pt_X9_YpOez4rO-fHxZl0T96Y#OWL	currently in use			See Declaration I1a.
I2 MD	eNanoMapper ontology	http://purl.org/np/RAGVk8evrODJcvukhw3d74EG_DeKU90r9uyfUlHNAwlOI#eNM	currently in use			Major activity of the nanosafety community to cover all data for risk assessment.
I2 MD	Elementary Multiperspective Material Ontology	http://purl.org/np/RAG_WQ6LruDpmtuhfQpS2IsIcf2gtSBTKJM9FbdCeg3z0#EMMO	planned use			Better alignment with the material modelling and characterisation communities is needed, which might be supported by the adoption of the EMMO. However, clearer concepts on how to annotate the MODA/CHADA reporting standards, potentially as part of the iMODA/iCHADA developments, need to be developed.
I2 D	eNanoMapper ontology	http://purl.org/np/RAGVk8evrODJcvukhw3d74EG_DeKU90r9uyfUlHNAwlOI#eNM	currently in use			See Declaration I2a.
I2 D	Elementary Multiperspective Material Ontology	http://purl.org/np/RAG_WQ6LruDpmtuhfQpS2IsIcf2gtSBTKJM9FbdCeg3z0#EMMO	planned use			See Declaration I2a.

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R1.1 MD	CC BY 4.0 | Attribution 4.0 International	http://purl.org/np/RAQ__sGdY_Qc7l1O_zmn4nr-pMBOxKU04Ur9s998rS6Fc#CC-BY-4.0	currently in use			This is the recommended license. However, journals and some databases might allow or require other licenses. Additionally, embargo periods are often enforced.
R1.1 D	CC BY 4.0 | Attribution 4.0 International	http://purl.org/np/RAQ__sGdY_Qc7l1O_zmn4nr-pMBOxKU04Ur9s998rS6Fc#CC-BY-4.0	currently in use			This is the recommended license. However, journals and some databases might allow or require other licenses. Additionally, embargo periods are often enforced.

Since we generated the initial FIP, the FIP Wizard has been updated and now includes the options to provide some further justification for the choices made, and some considerations on how the specific FER might be applied in different circumstances / cases. The WorldFAIR Nanomaterials FIP has been rolled over to Version 3.0 of the Wizard but we have yet to add the detailed considerations, including the reflections presented in Section 4, to the 'As-Is' FIP.

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4. Reflections on the initial Nanomaterials FIP: gaps and challenges

Some of the other WorldFAIR case studies have already prepared reports on their data management practices and policies and how these are documented in the corresponding FIPs (e.g., WP06 – Social Surveys[33], WP05 - Geochemistry[34], WP11 - Ocean Science and Sustainable Development[35], and WP13 - Cultural Heritage[36]). While most focus on listing and discussing the declared FERs and FSRs as implemented in their communities or specific data initiatives, platforms or services, WorldFAIR Deliverable D11.1, "An assessment of the Ocean Data priority areas for development and implementation roadmap"[37] stands out as it reviews all WorldFAIR Case Studies and extracts insights from them on how interoperability conventions of the Intergovernmental Oceanographic Commission of UNESCO's Ocean Data and Information System (ODIS) could be extended to enable cross-domain (meta)data flows.

As part of this analysis, an external view was included on the implementation of the FAIR principles in the Case Studies, as reported in the corresponding FIPs at the point of writing of the D11.1 report (March 2023). The statements made on WP04 provide a good starting point for discussing approaches, which are mentioned also in other FIPs and would therefore facilitate cross-domain interoperability when implemented broadly in the nanomaterial data resources.

4.1 Findability

D11.1 states that the Nanomaterials FIP reports a "balanced range of domain-neutral and domain-specific PID [permanent identifier] and/or more transient identifier maintenance systems"[38]. This needs to be clarified by looking at three different use cases for PIDs.

When defining the essence of the Findability principle as that "*(meta)data has been assigned unique and persistent identifiers and that those PIDs are linked to sufficiently 'rich' metadata to make them discoverable through expected search behaviours, and both the PIDs and their metadata are indexed in a reliable and searchable resource (e.g., a web-accessible repository)*", as done in Buttigieg et al. (2022), PIDs are used or are planned to be used in the nanosafety field mainly for dataset-level metadata on provenance (making the first use case). Digital Object Identifiers (DOIs) are, besides providing references to scientific publications supported by the dataset, used as globally unique and persistent identifiers for the dataset itself (e.g., DataCite DOIs via indexing in Zenodo). In most cases, these are generated additionally to the database-internal identifiers (if they are used at all). Data(set) citation still often relies on the internal identifiers assigned by the database storing the data (e.g.,, a GEO tag for omics datasets). Since the eNanoMapper database

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[33] https://zenodo.org/record/7584438
[34] https://zenodo.org/record/7380947
[35] https://zenodo.org/record/7682399
[36] https://zenodo.org/record/7659002
[37] https://zenodo.org/record/7682399#.ZFmcl87MK3A
[38] https://zenodo.org/record/7682399#.ZFmdeM7MK3A, p. 18.

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system (Jeliazkova et al., 2015) was, and probably still is, the most frequently used platform for providing data from European nanosafety projects, it is considered by many researchers that using the eNanoMapper identifiers and the eNanoMapper search interface is sufficient to get access to metadata. However, diversification of the database landscape, the current transition to 'Safe and Sustainable by Design'[39] and advanced materials and the even broader cross-domain interoperability goals, need the implementation of repositories covering the complete material data ecosystem. Additionally, full compliance with the FAIR principles demands independent access to metadata even if the data are not publicly available or not available any more. A domain-specific solution to these issues was created in the form of the NanoCommons Knowledge Base, which allows access to and searching of metadata from different database solutions including the NanoCommons Data Warehouse and all databases based on the eNanoMapper system. Another option is the general introduction of DOIs and the use of the services offered (e.g., by DataCite) as a domain-independent solution easily extendable to many data warehouses, institutional data repositories and data provided as supporting information in data journals, but this will require harmonisation and standardisation of at least high-level (dataset-level) metadata (see 'Interoperability' and 'Reusability' below).

Additionally, DOIs are proposed as qualified references to other supporting digital objects like corresponding method descriptions, protocols or even protocol steps, chemical reactions and (starting) materials. To uniquely identify persons and institutions as well as the projects and funding agencies as part of the provenance trail, standard identifiers and corresponding repository services like Open Researcher and Contributor ID (ORCID), Research Organization Registry (ROR) or International Standard Name Identifier for an identity (ISNI), DOIs for projects as provided by the European Commission, and the Crossref Funder Registry are proposed. At least ORCID and ROR are mentioned in many other WorldFAIR FIPs and are therefore recommended as highly relevant FERs for the WorldFAIR cross-domain interoperability framework[40]. Unfortunately, fully profiting from the project-specific identifiers is currently hindered by the fact that only the EU uses them, and as yet, no national funder provides DOIs for their projects. Additionally, the corresponding project-related metadata is not accessible via simple lookup services like the one provided by DataCite. Thus, users cannot integrate the metadata about the projects with other publications from official EU organs (e.g., EU Joint Research Centre[41], ECHA[42]) in tools like citation managers, by just specifying the DOI.

The second use case for PIDs is the annotation of metadata on a variable level, e.g., uniquely identifying specific experimental parameters. The nanomaterial and especially nanosafety

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[39] https://research-and-innovation.ec.europa.eu/research-area/industrial-research-and-innovation/key-enabling-technologies/chemicals-and-advanced-materials/safe-and-sustainable-design_en

[40] https://worldfair-project.eu/cross-domain-interoperability-framework/

[41] https://commission.europa.eu/about-european-commission/departments-and-executive-agencies/joint-research-centre_en

[42] https://echa.europa.eu/

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community is borrowing many identifiers from neighbouring communities and especially biology and chemistry. These include pathway, gene and protein identifiers (e.g., GO, Entrez, Ensembl, UniProt) and chemical identifiers (e.g., Chemical Abstract Service (CAS) Registry Numbers, European Community (EC) Numbers). The latter are also used as identifiers for the core component of nanomaterials, but covering the full complexity and separating different nanomaterials, also called nanoforms, with respect to size, shape and surface modification needs more specific identifiers. The EU Joint Research Centre created a repository of representative industrial nanomaterials[43] with a unique identifier for each material. Since these are distributed in support of the scientific community worldwide, these identifiers are referred to in many publications and datasets. However, many more materials are now subject to safety testing. To satisfy the need for being able to uniquely identify these, the European Registry for Materials (ERM) was created (van Rijn et al., 2022). Projects and individuals can register their materials and a unique identifier is provided. However, metadata available for these entries is unfortunately very limited / non-existing since only the project name is needed during registration. Information on the material can therefore only be collected by looking at resources (datasets, publications) referencing the identifier, which might lead to incorrect reuse of the identifiers when wrongly assuming identity. A similar situation is seen with the CAS Registry Numbers, where confusion is caused by multiple numbers assigned to the same chemical compound and groups of compounds only assigned to a single number.

Finally, the third use case for PIDs is specifically about identifying materials, even if the identifiers used do not fully comply with the essence of the 'Findability' principle as stated above. The simplified molecular-input line-entry system (SMILES and especially its canonical form), and the IUPAC International Chemical Identifier (InChI)[44] and its extension to nanomaterials (InChI for nanomaterials[45] or NInChI; see also Lynch et al., 2020) are line representations of chemical and nanomaterials structures, which can also be used as unique identifiers. But instead of relying on a repository service for providing information about the object associated with the identifier, the identifiers encode this metadata themselves. Different software packages are able to create the full chemical structure from SMILES and InChIs even if some details might be unspecified (e.g., exact stereochemistry, tautomeric state in InChI since this representation is meant to represent all possible tautomers). In a similar way, the NInChI is currently being developed to represent a group of nanoparticles. Even if there are experimental methods for characterising a single particle, such groups are the sensible option to describe materials, which are not formed out of identical particles but need to be represented by average values e.g., for size and/or by their distributions (see Blekos, et al., 2023).

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[43] https://joint-research-centre.ec.europa.eu/scientific-tools-and-databases/jrc-nanomaterials-repository_en

[44] https://www.inchi-trust.org/about-the-inchi-standard/

[45] https://www.inchi-trust.org/inchi-working-groups/#nano

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4.2 Accessibility

Due to the omnipresence of cloud- and web-based solutions for public as well as internal data management, the 'Accessibility' principle and especially the request for standard communication protocols are more or less completely addressed by standard web protocols such as HTTPS, FTP, and other TCP/IP protocols, alongside protocols used by contemporary Application Programming Interfaces (APIs) like representational state transfer (REST) and simple object access protocols (SOAP). Therefore, cross-domain interoperability is not really an issue here. Similar statements can be made for authentication and authorisation (A&A) and metadata preservation. Most data resources implement A&A even if the metadata and data is meant to be shared publicly. This allows embargo periods as well as monitoring of data access. Even if earlier versions of databases implemented custom-made solutions, they are now switching to standard solutions like OAuth, OpenID Connect and Keycloak and the implementation of single-sign-on and credentials provided by identity providers like EOSC/ELIXIR, Zenodo, ORCID and Google. Metadata preservation policies are also highly harmonised and guided by recommendations provided by funding agencies, within data management tools or by data registries like Zenodo. However, a decoupling of data and (high-level) metadata is, in most cases, implemented only for providing the information for the specific search features of a data resource but not for indexing of the metadata in relevant repositories. One exception is the NanoCommons Knowledge Base already mentioned above, which indexes metadata from other databases like eNanoMapper. This is still a completely domain-internal solution and cross-domain interoperability would need provision of metadata on a higher level.

4.3 Interoperability

Even if this sounds counterintuitive, the FERs used to address the 'Interoperability' principles are the least harmonised within the nanosafety community and the shifting focus to 'Safe and Sustainable by Design' and advanced materials has made it even more important to start the harmonisation of harmonisation processes. This is because strong collaboration and data exchange with the material modelling, materials characterisation and life-cycle assessment (both environmental and social) communities are absolutely essential for addressing the challenges. These communities developed their data management practices independently in the past based on different and partly incompatible high-level concepts.

When looking at knowledge representation languages, examples such as OWL, RDF and JSON(-LD) can be listed for the nanomaterials/safety community. However, this is not drawing an accurate picture since, even if these solutions are used, much of the data exchange and sharing in practice is still based on customised spreadsheets in CSV or even XLS format. The issue here is not that these solutions cannot be made FAIR but that they are often based on templates, which are specific to one project and are not described in a way that allows machine interoperability or reuse by others. This shows in the answers to the questions about the semantic models for metadata records and datasets. "Standard data curation formats/files", where 'standard' often only refers to a project-internal consensus (e.g., NANoREG, NIKC/NanoFASE, ASINA templates) or "bespoken models for individual databases" (e.g., eNanoMapper data model and the eNanoMapper template wizard

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creating mappings to this model) are very prominent but, because of their project/database-dependent origin, they are rarely adopted by others. ISA-TAB-nano and recently MODA/CHADA have been defined as (quasi)standards but have been adopted by very few projects and then only partly in a modified/simplified form. Incomplete coverage of the terminology needed for semantically describing the (meta)data additionally hampers interoperability. The eNanoMapper and EMMO ontologies, together with domain ontologies building on top of EMMO, are constantly developed to enlarge the coverage. However, there are many "standard" vocabularies used and/or developed in past and ongoing projects (e.g., NIKC, ACEnano, NanoSolveIT, Gracious), which are currently not FAIR themselves and thus cannot be classified as a FER for general usage by the community. Integration of these in existing ontologies is one of the most important tasks to be pursued as part of WorldFAIR.

4.4 Reusability

Specific FERs and FSRs can be assigned only to the licensing and provenance aspects of the reusability principle in the FIP wizard. For the first, the community is pushing for the implementation of the EU guidelines of "as open as possible, as closed as necessary" (e.g., by using Creative Commons licences) even if long embargo periods and not openly releasing metadata for all, even confidential data are strongly reducing re-usability.

In contrast, no clear and generally accepted guidance for provenance reporting is available for nanomaterials safety. This is part of a bigger issue that FAIR is assuming that community standards or best practices for data archiving and sharing exist and these have just to be acknowledged by agreeing to the standard declaration for R1.3. Even if the nanosafety community has been defining such practices for a long time, the result has been, on one hand, minimal reporting standards (e.g., MIRIBEL (Faria et al., 2018) and CODATA UDS), completeness checks and FAIR maturity indicators. But these are describing the reporting needs on a very high and scientific level by, e.g., specifying which characteristics have to be provided to clearly define a nanomaterial. On the other hand, too many "standards" implemented in project- or database-specific curation and upload templates were created without a computer- or even human-readable and easily accessible description of the implemented (meta)data model. This makes it almost impossible to compare the (meta)data models and document their evolution over time when handing them over from one project to the next. Interoperability and, thus, inter- and cross-domain re-usability would strongly profit from being able to automatically map different (meta)data models onto each other based on specification describing the (meta)data fields and their relationships. Standard ways to generate such specifications are implemented e.g.,, in DDI Codebook and DDI Lifecycle. Requesting that all nanomaterial data resources provide now a full specification of each partly dataset-specific (meta)data model will be almost impossible and, even if everyone could be convinced, would take a very long time to be completed. Therefore, concentration on the most important (meta)data fields and starting with their harmonisations will bring benefits faster and improve many aspects of FAIRness. Guidance for the selection of these fields can be taken from standards like Dublin Core, the DataCite metadata schema, W3C'sPROV specific for provenance data, and the DLite approach to data integration and promoted by the EMMC. Even if these only cover parts of the (meta)data

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model and especially the dataset-level metadata, building the model from these pieces would directly guarantee cross-domain interoperability on this high level relevant for finding and accessing the data.

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5. Next steps and ongoing work

5.1 FAIR convergence mapping

The WorldFAIR nanomaterials FIP has been integrated into the ongoing PARC FAIR convergence analysis, as well as the PARC activity to verify all of the declared FERs from the FIPs developed in WorldFAIR and in PARC. Thus, the FAIR Implementation TaskForce in PARC (of which the UoB team are members) are now sufficiently far into their GO FAIR 3-point FAIRification Framework[46] training to be authorised to validate the FAIRness of declared FERs, utilising an agreed process.

Based on the outcomes of the verification process, the next steps to increase the FAIRness of the resources declared as supporting or enabling in the Nanomaterials FIP will be actioned to increase their FAIRness further – this can include, for example, declaring them in FAIRsharing.org, confirming that all hyperlinks work, or that the type of resource has been correctly defined.

5.2 Building data management workflow engines with KNIME for FAIR data

A key next step for WP04 in WorldFAIR is to build FAIR data management workflows engines within KNIME (Figure 6) to enable FAIRification of data by developing a library of common services and building blocks for FAIR data workflows using KNIME, tailored to nanomaterials databases, ontologies, metadata schema and more. This library will include predefined workflows for common data management tasks and building blocks, as well as tools for managing data provenance, metadata, and quality. The task will also develop methods for integration of external tools and services into KNIME workflows to increase the granularity and flexibility of the workflows, including development of custom nodes for integrating external tools and services into KNIME workflows.

As part of the documentation and testing phase, the FAIR data workflows will be evaluated to ensure that they are robust, efficient, and effective. This testing will involve a combination of manual testing and automated testing using tools such as unit testing frameworks and integration testing tools. Additionally, the effectiveness of the FAIR data workflows will be evaluated by conducting user studies and obtaining feedback from domain experts. This evaluation will help to identify areas for improvement and further development.

Combining data from different Excel files into KNIME and transforming it into FAIR data involves several key steps, as shown schematically in Figures 7 and 8. By following these steps, the disparate data from multiple sources can be integrated, standardised, and made FAIR-compliant:

1. *Data import and consolidation*: To start, import the data from multiple Excel files into KNIME using appropriate Excel Reader nodes. Once the data is imported, it can be combined using nodes such as Concatenate, Joiner, or Merge, depending on the desired outcome and the structure of the input data (Figure 7).

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[46] https://www.go-fair.org/2020/07/08/a-three-point-framework-for-fairification/

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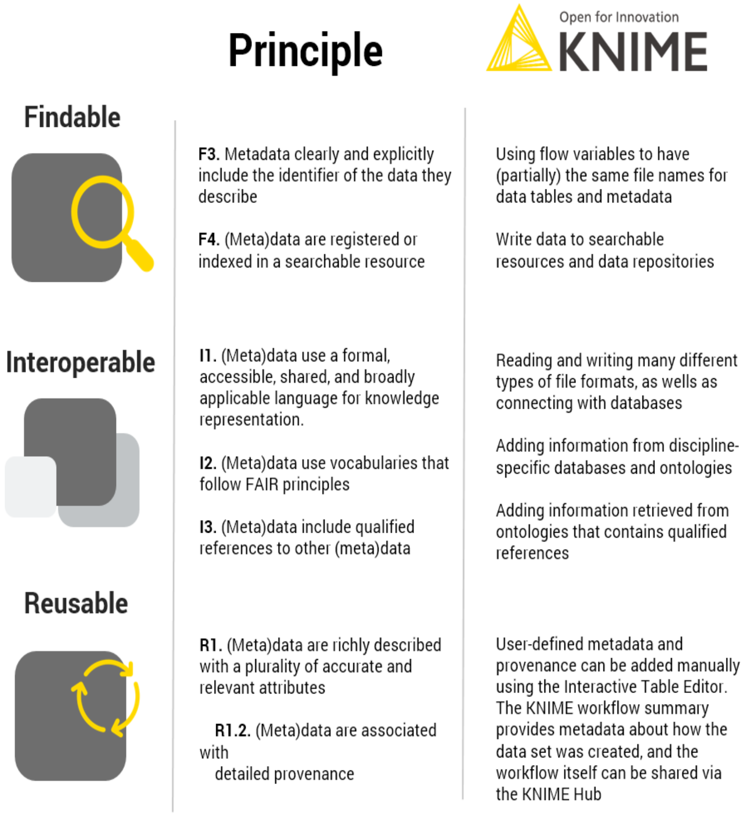
2. *Data preprocessing and cleaning*: Before transforming the combined data into FAIR data, it's essential to preprocess and clean it. This may involve removing duplicates, filling in missing values, correcting inconsistencies, and normalising data formats. Use nodes like Missing Value, Duplicate Row Filter, Row Splitter, and String Manipulation to address these issues.
3. *Metadata enrichment*: For data to be FAIR, it should be accompanied by rich and structured metadata. Use nodes like Column Properties, Column Rename, and Column Filter to add, modify, or remove metadata, such as descriptions, units, or data types, as needed.



	Principle	Open for Innovation KNIME
Findable	**F3.** Metadata clearly and explicitly include the identifier of the data they describe **F4.** (Meta)data are registered or indexed in a searchable resource	Using flow variables to have (partially) the same file names for data tables and metadata Write data to searchable resources and data repositories
Interoperable	**I1.** (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation. **I2.** (Meta)data use vocabularies that follow FAIR principles **I3.** (Meta)data include qualified references to other (meta)data	Reading and writing many different types of file formats, as wells as connecting with databases Adding information from discipline-specific databases and ontologies Adding information retrieved from ontologies that contains qualified references
Reusable	**R1.** (Meta)data are richly described with a plurality of accurate and relevant attributes **R1.2.** (Meta)data are associated with detailed provenance	User-defined metadata and provenance can be added manually using the Interactive Table Editor. The KNIME workflow summary provides metadata about how the data set was created, and the workflow itself can be shared via the KNIME Hub

Figure 6. FAIR aspects that KNIME can contribute to (image from: https://shorturl.at/grCFL).

4. Data standardisation: FAIR data should adhere to standardised vocabularies, formats, and identifiers. Depending on the domain, apply appropriate standardisation nodes (e.g., Ontology-based Data Standardization) to ensure consistency in terms, units, and formats used in the dataset (Figure 8).
5. Data provenance tracking: Documenting the data's provenance is a key aspect of FAIR data. Utilise nodes that capture data transformation history and provide an audit trail for each step in the workflow.

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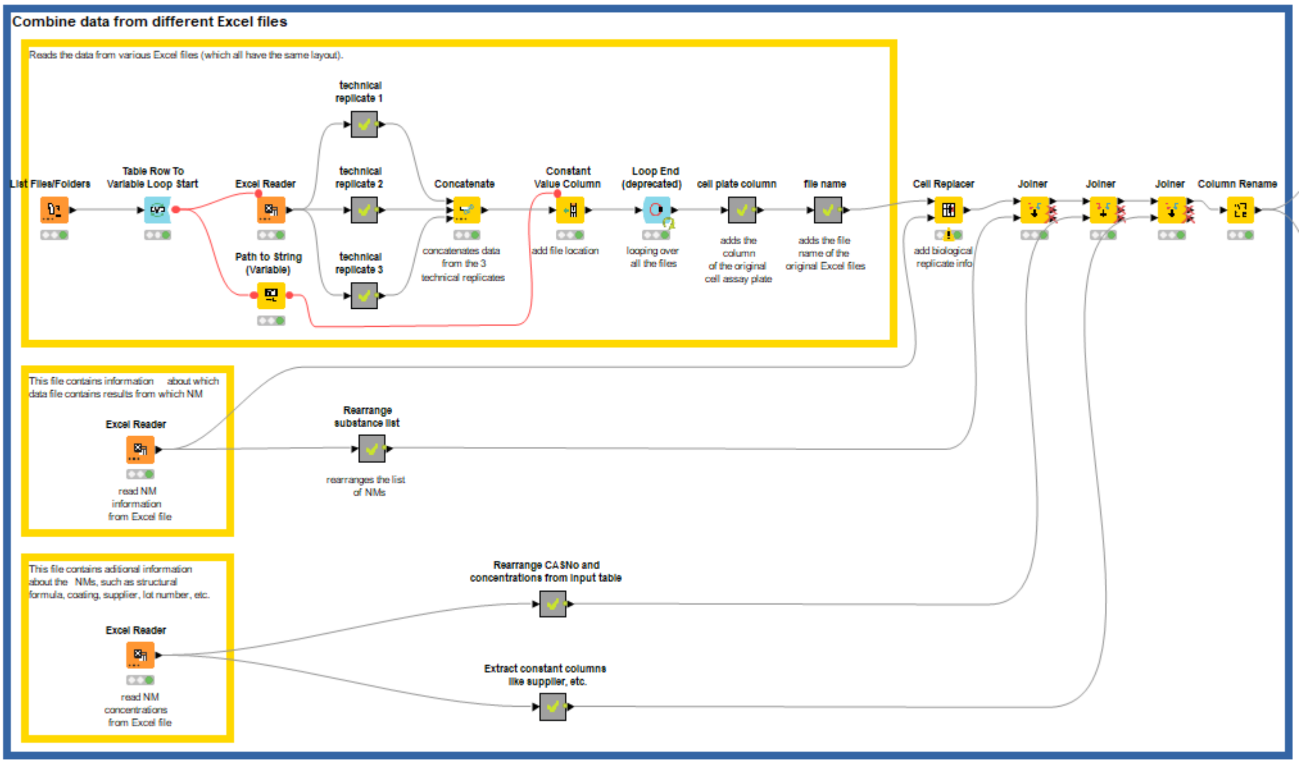
6. Data export and sharing: Once the data has been transformed into FAIR data, export it into a suitable format (e.g., CSV, JSON, RDF) using appropriate Writer nodes. Share the data on platforms that support FAIR principles, such as open data repositories, to ensure it is findable, accessible, and reusable by others.
7. Workflow documentation and sharing: document the KNIME workflow used to transform the data into FAIR data, including the nodes and configurations. Share the workflow, along with instructions on how to use it, to enable others to adopt the FAIR data practices in their own projects.



Combine data from different Excel files

Reads the data from various Excel files (which all have the same layout).

This file contains information about which data file contains results from which NM

This file contains aditional information about the NMs, such as structural formula, coating, supplier, lot number, etc.

Figure 7. Combining data from different Excel files - representative workflow. Note that the full-size image (which can be "zoomed in" to see the details) is available on the [KNIME website]() and also lists the specific nodes that were utilised in the demonstration case.

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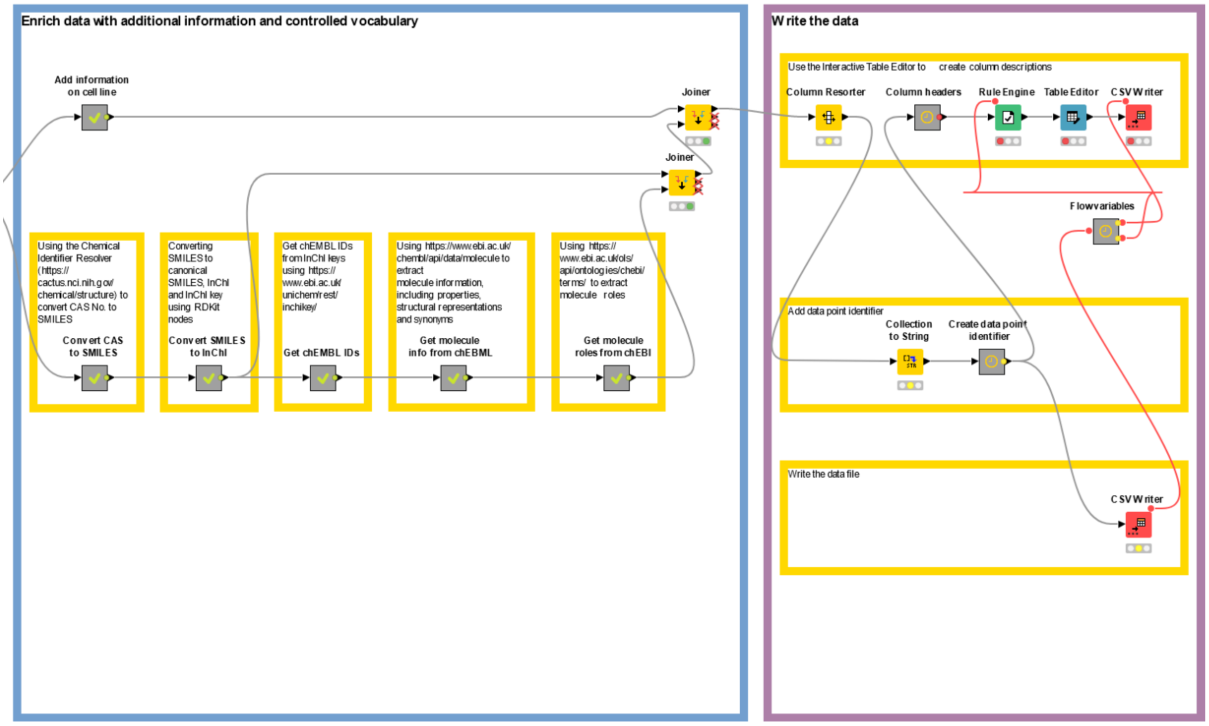

Figure 8. Enriching the data with controlled vocabularies and additional information such as identifiers (E.g. InChI) using a representative KNIME workflow. Note that the full-size image (which can be "zoomed in" to see the details) is available on the [KNIME website](#) and also lists the specific nodes that were utilised in the demonstration case.

An example case study, focused on nanomaterials, which aims to enrich the current data with additional information and controlled vocabularies using KNIME, while adhering to the FAIR data principles, will be utilised to demonstrate the FAIR nanomaterials workflow. The integration of external data sources such as ChEMBL and PubChem into data management workflows can provide valuable information about the properties and characteristics of the nanomaterials. The procedure was started by importing nanomaterial data into KNIME using appropriate Reader nodes, based on the input file format. The next step was identification of the columns in the dataset that require enrichment with controlled vocabularies or ontologies, such as terms from ChEMBL or PubChem, to improve data interoperability. Next, we have acquired the controlled vocabularies and additional information from ChEMBL and PubChem using GET Request or RESTful Web Services nodes. Then integration of this information with the original dataset using nodes like Joiner, Concatenate, or Merge, depending on the structure of the external data and the desired output. To standardise the data, we have applied the controlled vocabularies or ontologies from ChEMBL and PubChem to the relevant columns of the dataset. This involved matching terms, replacing existing terms with standardised ones, or adding new columns to represent the mapped terms. Nodes like Rule Engine, String Manipulation, or Column Rename are used to perform these operations. Afterwards, we have updated the metadata for the enriched columns to reflect the new information, controlled vocabularies, or ontologies applied, using Column Properties or Column Rename nodes. The next

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step was the validation and cleaning of the enriched data, ensuring consistency and accuracy by removing duplicates, handling missing values, and correcting inconsistencies with nodes like Missing Value, Duplicate Row Filter, or String Manipulation. Once the data has been cleaned and validated, we have exported the enriched, FAIR-compliant data using suitable Writer nodes and shared them on platforms that support FAIR principles, such as open data repositories. The KNIME workflow can be documented and shared along with instructions on how to use it, encouraging the adoption of FAIR data practices in other nanomaterial-focused projects.

By enriching nanomaterial data with additional information and controlled vocabularies from ChEMBL and PubChem, and following FAIR principles using KNIME, WorldFAIR researchers can create standardised, interoperable, and reusable data procedures. This contributes to more efficient and collaborative research practices within the nanomaterials research community.

One challenge that will need to be addressed is the creation of robust FAIR data workflows in advance of fully knowing the data. To address this, the project will focus on developing a library of common services and building blocks to facilitate the creation of FAIR data workflows. Additionally, file-based workflow systems may not be granular enough for FAIR data workflows, so the project will focus on developing methods for integrating external tools and services into KNIME workflows to increase their granularity and flexibility.

5.3 FAIRifying nanoinformatics models

5.3.1 Exposure simulations and integrated approaches for nanomaterials safety assessment

Integrated approaches to testing and assessment (IATA) have emerged as a valuable framework for combining experimental and *in silico* data for hazard characterisation of chemicals, including nanomaterials. Experimentally acquiring the necessary exposure, hazard, and characterisation data for nanomaterials to perform risk assessment is both time-consuming and costly. In response, *in silico* models have gained traction for facilitating read-across from data-rich nanomaterials to data-poor ones and for predicting exposure or hazard.

In a recent work (Tsiros et al., 2021), three integrated computational approaches have been developed to generate data relevant to human health risk assessment:

1. The multi-box aerosol model predicts indoor air concentrations of nanomaterials by simulating the movement, deposition, and clearance of aerosols in indoor environments, considering factors such as aerosol source strength, room size, ventilation rate, and particle size distribution.

2. The lung exposure model, based on empirical deposition equations, calculates the deposited mass in different regions of the human respiratory system (e.g., alveolar, tracheobronchial, and head airways) to determine the lung burden of nanomaterials following acute exposures.

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3. The physiologically-based pharmacokinetic (PBPK) model builds upon the lung exposure model by introducing clearance terms and translocation of nanomaterials to the systemic circulation after passage through the air-blood barrier in the alveoli, allowing the determination of the biodistribution of nanomaterials to other organs over longer timescales following inhalation exposure.

These models can be applied to a variety of exposure scenarios with different conditions, enabling the comparison of the models concerning the accumulated mass of nanomaterials in different regions of the respiratory system. This comparative approach allows researchers to explore the capabilities and weaknesses of each model and their potential contributions to a nanomaterial-specific IATA for occupational exposure. The widespread use of nanomaterials in daily life highlights the need for understanding their long-term and cumulative impact on human health. However, experimental methods for studying their biodistribution and clearance are expensive and ethically challenging, leading to limited data on specific nanomaterials and reliance on rodent models. Computational tools provide a promising solution for assessing the impacts of nanomaterials exposure on humans. The proposed integrated computational framework assesses the internal deposition and distribution of nanomaterials following exposure in an occupational setting, connecting an external exposure model with internal exposure models for acute and chronic timescales. This integrated approach enables users to conduct a comprehensive *in silico* environmental risk assessment. Furthermore, the computational methodology for calculating the spatiotemporal emission profile can be extended to encompass nanomaterial emissions to the surrounding environment in addition to indoor exposure, enhancing the scope of *in silico* environmental risk assessments.

In the particular work, the integrated computational approaches for nanomaterials safety assessment were developed in line with the FAIR principles to ensure that the data generated and used are easily discoverable, accessible, interoperable, and reusable for other researchers and stakeholders.

5.3.2 Increasing FAIRness of Computational Hazard Assessment models

In a collaborative effort by WorldFAIR participating partners, a study on predicting cytotoxicity of metal oxide nanoparticles (MexOy nanoparticles) using the Isalos Analytics Platform[47] has been conducted (Papadiamantis et al., 2020b). This project underscores the importance of the FAIR concept, ensuring that the data and tools generated can be easily discovered, accessed, and used by researchers worldwide. The study utilised a literature-curated dataset containing 24 distinct MexOy NPs, enriched with 15 physicochemical, structural, and assay-related descriptors along with 62 atomistic computational descriptors. The resulting dataset was used to develop a robust and validated *in silico* model to predict nanomaterial cytotoxicity. The cytotoxicity predictions were based on two assays: the colorimetric lactate dehydrogenase (LDH) assay and the luminometric adenosine triphosphate (ATP) assay, which both quantify irreversible cell membrane damage. Out

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[47] https://isalos.novamechanics.com/

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of the 77 total descriptors employed, the study identified seven significant factors for inducing cytotoxicity in MexOy nanomaterials: nanoparticle core size, hydrodynamic size, assay type, exposure dose, energy of the MexOy conduction band (EC), coordination number of metal atoms on the nanoparticle surface (Avg. C.N. Me atoms surface), and average force vector surface normal component of all metal atoms (v⊥ Me atoms surface). The study discusses the significance and effect of these descriptors, demonstrating their direct correlation with cytotoxicity. The *in silico* model generated in this study is publicly available as part of the Horizon 2020 (H2020) NanoSolveIT project, and will be incorporated into the project's IATA. The model provides a valuable tool for predicting MexOy nanoparticle cytotoxicity, allowing for read-across based on chemical similarity and utilisation of the LDH or ATP assays. By adhering to the FAIR principles, the researchers of this project have ensured that the curated dataset, which includes values for Avg. C.N. Me atoms surface and v⊥ Me atoms surface, is easily accessible through the NanoPharos[48] database. Moreover, the developed model is publicly available as a web service via the NanoSolveIT Cloud Platform[49], promoting transparency and fostering collaboration among researchers who are studying nanomaterial safety. To thoroughly demonstrate that the generated cytotoxicity model meets the OECD criteria, the researchers have included a completed QSAR Model Reporting Format (QMRF) template in the Supplementary Information section of their study. By providing this information, they offer a comprehensive report on the quality and reliability of the model, enabling other scientists to assess its applicability and usefulness in predicting the cytotoxic effects of metal oxide nanoparticles. This commitment to transparency and open sharing of information is a testament to the researchers' dedication to advancing the field of nanomaterial safety through adherence to the FAIR principles.

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[48] https://db.nanopharos.eu/

[49] https://cloud.nanosolveit.eu/

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Appendix 1: The ‘As-Is’ Nanomaterials FIP – Version 1 – extended document

FAIR Principl name	**Referring to MetaData / Data**	**FIP question**	**Type of FAIR Enabling Resource**	**FER Type definition**	**FER Enabling Resource used in WP04 Nanomaterials**	**FAIRshairing DOI**	**URL**	**Status of Use (Current, To Be Replaced, Future)**	**Implementation Considerations**	**Comments**
F1.1	MD	What globally unique, persistent, resolvable identifier service do you use for metadata records?	identifier service	A **service** that provides for metadata (1) algorithms guaranteeing global uniqueness, (2) policy document that guarantees persistence and (3) resolution of the identifier to machine-actionable metadata describing the object and its location.	DataCite DOIs	N/A?	https://datacite.org/dois.html	Current	In some datasets, data and metadata are largely combined in the dataset.	Example: https://nanocommons.github.io/datasets/ Partial implementation
					InChI? Institutions, People?	[10.25504/FAIRsharing.ddk9t9](https://doi.org/10.25504/FAIRsharing.ddk9t9)	https://www.inchi-trust.org/	Future		
					NanoInChI		http://www.enaloscloud.novamechanics.com/nanocommons/NInChI/	Future		

FAIR Principl name	**Referring to MetaData / Data**	**FIP question**	**Type of FAIR Enabling Resource**	**FER Type definition**	**FER Enabling Resource used in WP04 Nanomaterials**	**FAIRshairing DOI**	**URL**	**Status of Use (Current, To Be Replaced, Future)**	**Implementation Considerations**	**Comments**
F1.2	D	What globally unique, persistent, resolvable identifier service do you use for datasets?	identifier service	A **service** that provides for data (1) algorithms guaranteeing global uniqueness, (2) policy document that guarantees persistence and (3) resolution of the identifier to machine-actionable metadata describing the object and its location.	DataCite DOIs	N/A	https://datacite.org/dois.html	Current		In use, but not community-wide
					DB specific unique identifiers	Per case	Per case	Current	Unique within scope of the database?	In many cases there is a lack of a harmonised, easy-to-use / reuse / publish identifier.
					Identifier with internal semantic meaning			Future	Desideratum	
F2	MD	What metadata schemas do you use for findability?	metadata schema	A **specification (schema)** that defines metadata fields describing attributes of data or other digital objects.	DataCite Core	https://fairsharing.org/FAIRsharing.me4qwe	https://schema.datacite.org/meta/kernel-4.4/doc/DataCite_D	Current, by using DataCite DOI		

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							ublinCore_Mapping.pdf			
					Dublin Core	10.25504/FAIRsharing.3nx7t	https://www.dublincore.org/	Future		There are some use, but cannot considered as current cause it is very limited within the community
					schema.org	https://fairsharing.org/FAIRsharing.hzdzq8	schema.org	Future	Used by some people in part of the domain	
					bioschema.org	collection: https://fairsharing.org/3517	bioschema.org	Future	Used by some people in part of the domain	Example: https://nanocommons.github.io/datasets/
					Frictionless Data			Future	Used for tabular data / csvs	
		hat is the schema that links persistent identifiers	etadata-data linking schema	**specification** that provides a unique, persistent, (ideally)	DataCite, Repository,	10.25504/FAIRsharing.yknezb	https://search.datacite.org/	Future	Link from repository metadata to data.	

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		of data to metadata description ?		bi-directional, machine-actionable link between metadata and the data they describe.	Some repos link to the article, or the shared authors			Future	Not really considered as in most cases the dataset is uploaded before the publication and linking does not really take place. Linking should happen via automating the repositories and their linking to identifiers like e.g.,, ORCID.	
.1	D	hich service do you use to publish your	gistry	**service** that indexes metadata and data and provides search over that index.	Zenodo	10.25504/FAIRsharing.wy4egf	https://zenodo.org/	Current		It is a go-to place as it is the easiest way to implement.
					Institutional Repository			Current/To be replaced	Mention specific IRs and add URL	While many Institutions require submitting data to internal repositories these

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		metadata records?								are not usually accessible from external users. As such, it is hard to categorise them as FAIR.
					DataCite		https://datacite.org/index.html	Future		Not widely implemented.
					NanoCommons Knowledge Base	https://fairsharing.org/2979	https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi	Current		Provide documentation.
					nanoPharos Database		https://db.nanopharos.eu/	Current		
					Peer Reviewed Article			Current		
					Data Journals?		https://www.sciencedirect.com/org/journal/iucrdata	Future	Increase knowledge within the community on the value of such journals.	Provide examples.

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					Wikidata					
.2		hich service do you use to publish your datasets?	gistry	service that indexes metadata and data and provides search over that index.	Zenodo	10.25504/FAIRsharing.wy4egf	https://zenodo.org/	Current		
					Figshare	10.25504/FAIRsharing.drtwnh	https://figshare.com/	Current		
					Institutional Repository			Current / to be replaced	Not external accessibility.	Institutions require adding your data and metadata within internal repositories.
					NanoCommons Knowledge Base	awaiting DOI: https://fairsharing.org/2979	https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi	Current		Provide documentation.
					Peer Reviewed Article and linked database			Current		

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					Data Journals?			Future		Provide examples.
1.1	D	Which standardised communication protocol do you use for metadata records?	ommunication protocol	**specification** that defines how messages are structured and exchanged.	http, https	[10.25504/FAIRsharing.cd2f9e]()		Current		As part of the URL used during publication in databases, journals etc.
					REST APIs			Current		
					SOAP			Current		
1.2		Which standardised communication protocol do you use for datasets?	ommunication protocol	**specification** that defines how messages are structured and exchanged.	http, https (unique URL with dataset ID e.g https://db.nanopharos.eu/Queries/Datasets.zul?datasetID=2)	[10.25504/FAIRsharing.cd2f9e]()		Current		
					ftp			Future		Very limited use.
					REST APIs			Current		
					SOAP			Current		

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2.1	D	hich authentication & authorisation service used for metadata records?	uthentication and authorization service	**service** that mediates access to digital objects according to specifed conditions	Metadata is generally open.			Current		Most common is embargo imposed by projects before sharing.
					EOSC / Elixir	https://fairsharing.org/3527 https://fairsharing.org/1089	https://eosc-portal.eu/ https://elixir-europe.org/	Current	Currently being more widely implemented.	
					Keycloak			Future		
					Registration SSO etc.			Future		
2.2		hich authentication & authorisation service used for datasets?	uthentication and authorization service	**service** that mediates access to digital objects according to specifed conditions	Case by case basis, some may use Shibboleth.			Current		Mainly used by journals and academia.
3.1	D	hat metadata preservation policy do you use?	etadata preservation policy	**document** that describes the conditions under which metadata are to be provisioned in the	Zenodo's policy by implication.			Current	Doubtful that users read it	
					Institutional or funder DMP requirements, DMPonline		https://dmponline.dcc.ac.uk/	Current		

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				future (generally part of a data management plan).	FAIR Stewardship Wizard (GO FAIR)		https://ds-wizard.org/	Future		
					EOSC / OpenAire DMP tool - Argos		https://argos.openaire.eu/home	Future		
.1	D	hat knowledge representation language (machine interoperation) is used for metadata records?	owledge representation language	language **specification** whereby knowledge can be made processible by machines.	OWL	10.25504/FAIRsharing.atygwy		Future		
					RDF	no DOI yet: https://fairsharing.org/336		Future		
					JSON (nanoPharos - REST APIs using JSON format)			Current	ISAtab expressed in JSON	
.2		hat knowledge representation language (allowing machine	owledge representation language	language **specification** whereby knowledge can be made processible by machines.	OWL	10.25504/FAIRsharing.atygwy		Future		Describe role of AberOWL
					XLS			Current		
					CSV (is safer for data upload)			Current		
					JSON			Current		

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		interoperation) do you use for datasets?			JSON-LD			Current		
					ISAtab Nano			Current		This is not used a lot.
					Simplified JRC / NanoREG templates			Current		
					Mass spectrometry binary data files			Current		
					RDF	no DOI yet: https://fairsharing.org/336		Current		
.1	D	hat structured vocabulary do you use to annotate your metadata records?	ructured vocabulary	**specification** of uniquely identified and unambigous concepts with their definitions represented preferably using web standards.	NanoInChI (conceptually this is a classification)			Future		
					Reuse of life sciences vocabularies.			Future		
					NIKC (sp?) vocabulary			To be replaced		Limited use within the NIKC database. Not expected to be used more widely.
					NanoReg vocabulary			To be replaced		

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					eNanoMapper ontology		https://www.enanomapper.net/ontology	Current	Currently being maintained / extended under the inheritance umbrella of publicly funded projects. Restructuring is required to rectify identified issues.	
					new terminologies based on physics based simulations (currently not included under a specific ontology)			Future	Very specialised work that requires expert knowledge and definition.	
					ISO Terms		Link to specific products.	Future		
					EMMO (Elementary Multiperspective Material Ontology)		https://github.com/emmo-repo/EMMO	Future		

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					New terminologies/descriptors for nanomaterials properties.			Future		Antreas to provide some examples, links.
.2		hat structured vocabulary do you use to encode your datasets?	ructured vocabulary	**specification** of uniquely identified and unambiguous concepts with their definitions represented preferably using web standards.	NanoInChI (conceptually this is a classification)			Future	Under development. Needs to be introduced to the wider community.	
					Willighagen work on material identfiers? (ditto)			Current		
					eNanoMapper ontology	[10.25504/FAIRsharing.2gpf81]()		Current		
.1	D	hat semantic model do you use for your metadata records?	mantic model	**specification** that defines qualified relations between entities describing data or other digital objects using structured vocabularies.	ISATab			Current		
					eNanoMapper ontology	[10.25504/FAIRsharing.2gpf81]()		Current		Consult with Egon Willighagen
					Reuse of life scineces ontologies.			Future		

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					EMMO (Elementary Multiperspective Material Ontology)		https://github.com/emmo-repo/EMMO	Future		
.2		'hat semantic model do you use for your datasets?	mantic model	**specification** that defines qualified relations between entities describing data or other digital objects using structured vocabularies.	Standard data curation format files.			Future	Wider community discussions and consensus are required.	
					Bespoke models for individual databases			Current	While these exist, mapping between them is required to establish communication and increase FAIRness.	
					NanoForms			Current		Regulatory reporting requirements.
.1	D	'hich usage licence do you use for your metadata records?	ta usage licence	**document** that describes the conditions under which a digital object can be legally used.	CC (which flavour?)					See for used examples: https://nanocommons.github.io/datasets/ s
					Zenodo default is CC-BY v.4					For how to use for CCZero: https://chem-bla-ics.blogspot.com/2022/09/how-to-m

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										ark-something-cczerocc0-on.html
					Default licence from journal			Current	The default option currently.	Some are horrible, like "CC-BY OR CCZero, and you have to guess"
1.2		hich usage licence do you use for your datasets?	ta usage licence	**document** that describes the conditions under which a digital object can be legally used.	Zenodo default is CC-BY v.4			Current	Mainly used for resources uploaded to Zenodo.	See https://chem-bla-ics.blogspot.com/2022/09/how-to-mark-something-cczerocc0-on.html for how to use CCZero
					Default licence from journal			Current	Default option currently.	Some are horrible, like "CC-BY OR CCZero, and you have to guess"
					Complex ownership arrangements in consortia			Future	Now being implemented within certain projects. Will eventually become the standard in Europe	

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									due to EU requirements. Needs to be established from the onset, as it is a long and hard to agree procedure.	
2.1	D	hat metadata schema is used to describe provenance of metadata records?	ovenance model	**specification (schema)** that defines metadata fields describing the origin and lineage of data or other digital objects.	CODATA UDS			Future		
					Bioschemas	collection: https://fairsharing.org/3517		Current		
2.2		hat metadata schema do you use for describing the provenanc	ovenance model	**specification (schema)** that defines metadata fields describing the origin and lineage of data or other digital objects.	CODATA UDS			Future		
					ISAtab			Current		
					Bioschemas	collection: https://fairsharing.org/3517		Current		Any use of PROV-O?

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		e of your datasets?			Functions in eMR (eMaterials Registry)			Future		
					Instance Maps		Reference papers:. (https://www.mdpi.com/2079-4991/10/10/1936 Figure1); https://ncihub.cancer.gov/resources/2153/download/CEINT_NIKC_DataDictionary_20180531.pdf	Future	Not widely implemented. Currently under development based on the work by NIKC.	Developed by Duke, implemented by 7P9; links various stages in use of nanomaterials

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