

Article

Data Shepherd in Nanotechnology: An Antimicrobial Functionality Data Capture Template

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Abstract: In this paper, we exhibit how to construct a template for capturing antimicrobial capacity data of nanomaterials or nanoenabled products. The template promotes the principles of making data scientifically findable, accessible, interoperable and reusable (FAIR), encouraging scientists to reuse it. The template construction roadmap entails the following steps: (1) recognize appropriate stakeholders, (2) allocate surveys to collect a general explanation of the data that will be created, (3) comprehend each stakeholder's requirements, (4) cooperating and using straightforward communication with the participants for the selection of the minimum data requirement reporting and (5) template layout and ontological annotation. We provide an annotated template for capturing antimicrobial data, increasing their interoperability while populating it with real measurements as an example. By applying the roadmap or by utilizing the template portrayed herein, in the case of a safe-by-design nanoproject (Anticipating Safety Issues at the Design of Nano Product Development (ASINA)), data creators of antimicrobial assessments can store the data using the FAIR approach. Furthermore, data shepherds and scientists can skip the lengthy template generation process and speed up the community's progress on the FAIR route.

Keywords: nanotechnology; antimicrobial; FAIR data; nanomaterials; coating

1. Introduction

Antibiotics are still being used as a medication for bacterial diseases and the inappropriate use of them has resulted in the evolution of bacterial resistance [1,2]. Multidrug-resistant bacteria's emergence and biofilm formation are a public health concern [3,4]. According to the World Health Organization, bacterial resistance is posing an increasing danger to global health and the achievement of sustainable development goals [5]; this growing issue necessitates the generation of long-term and efficient novel antimicrobial (and biofilm-preventing) materials. Consequently, attention has been devoted to relatively emerging fields such as nanotechnology and the development of nanoenabled finished multifunctional materials.

Nanomaterials (NMs) and their diverse nanoforms have enhanced properties in comparison to their bulk material, including antimicrobial efficacy toward a range of microorganisms [6]. The antimicrobial properties of NMs are superior, motivating their use as a viable alternative to antibiotics [7]. The study of NMs is of tremendous importance since they may be used in various disciplines, including medicine, food processing and

cosmetics, while still preserving their unique properties [8–11]. The search for innovative antimicrobial compounds has been crucial throughout the last few decades to various research fields for the reduction of nosocomial and foodborne infections [12–14]. Recent publications have reflected the increasing trend of manufactured products around the field of nanotechnology and the enhanced antimicrobial capacity of NMs for diverse healthcare applications [2].

In the realm of nanotechnology, machine learning (ML) techniques were used with favorable findings [15]. ML was shown to be helpful for acquiring insights into factors that affect toxicity, forecasting probable adverse effects and guiding safe-by-design paradigms [16,17]. The knowledge that is available through curated databases and the scattered available datasets from studies in the literature is mainly focused on human and environmental toxicological endpoints and physicochemical (p-chem) characterization data [18,19]. Emerging infrastructures are being developed, such as the EU-funded projects, NanoCommons <https://www.nanocommons.eu/> (accessed on 27 November 2021), GRACIOUS <https://www.h2020gracious.eu/v> (accessed on 27 November 2021) and eNanoMapper <http://www.enanomapper.net/> (accessed on 27 November 2021), to address the data quality and availability of existing data. NanoSolveIT <https://nanosolveit.eu/> (accessed on 27 November 2021) is assembling data from various sources and curating, merging and FAIRifying (assuring findability, accessibility, interoperability and reusability) existing and new data on the health and environmental safety of NMs. These FAIR principles acquired popularity in the scientific community and are expected to grow into the cornerstone of research policy and requirements for research data management plans [20]. The principles emphasize several important preconditions for data sharing, asking researchers to consider the prospect of future data sharing and reuse from the start [21]. Their simplicity and flexibility are significant assets, allowing for the formation of agreed goals and courses of action in research data management. As a result, the FAIR principles give a vital stimulus to data-driven research culture, allowing for transparent data reuse for accelerating nanotechnology research [21,22]. However, individual researchers and research organizations, as well as research communities, will have to rise to the occasion.

A significant number of studies that examined NMs' antimicrobial capacities exist in the literature. Antimicrobial assessments generate a large amount of data that are useful and indispensable for both research and industry. While a tremendous amount of data exists in the literature, there is no systematic and comprehensive source of data regarding antimicrobial capacity that provides all or most information in one place. Unfortunately, the antimicrobial data of NMs are not as readily available as data related to toxicological endpoints. In a study conducted by Mirzaei et al. [23], information from studies was manually extracted following a literature review regarding NMs that were introduced to diverse bacteria to measure the NMs' antimicrobial capacity. The aforementioned study revealed that very little information is included in the original studies, specifically the characterization data that reveal the key properties that enhance the antimicrobial capacity of NMs. Another finding of the study was the diversity of the reporting antimicrobial endpoints. Several endpoints of the same functionality were extracted and recorded, such as bacteria viability, minimum inhibitory concentration, zone of inhibition or colony-forming unit. The outcomes were expressed in different metrics, which were unable to be merged. This emphasized the need for a consistent method for antibacterial examinations, as well as a structured manner for reporting scientific data findings. The conclusion was that the information is scattered and incomplete and manual extraction of data is highly time-consuming and inappropriate.

In academia and industry, data is rarely leveraged for purposes other than those that were originally intended [24]. Technologies that follow and provide data that hold onto the FAIR principles are critical enablers of digital transformation [25]. FAIR data are imperative modules of the EU industrial strategy, chemicals strategy for sustainability and circular economy action plan, all of which are based on the EU Green Deal (https://ec.europa.eu/environment/strategy/chemicals-strategy_en (accessed on 27 Novem-

ber 2021), which fosters safe and sustainable by design (SSbD) frameworks and innovations [26,27]. The EU has increased its demand for open data research and has crafted FAIR data management guidelines for H2020 projects that create data and a data management plan as a required deliverable [28]. The FAIR data principles are specifically referenced in the appropriate guidelines. Given that a rising number of researchers will be exposed to the recommendations, it is critical to analyze their viability and suggest areas where they could be improved [20]. Data management refers to the full data implementation lifecycle, which includes the data production, collection, variation and final storage [29]. The principles of FAIR were discussed in depth in preceding scientific articles [21,25,30,31]. FAIR principles were created to outline good data management practices. What establishes good data management or stewardship is currently vague and it is frequently left to the discretion of the data creators and/or holders [30,32]. As Wilkinson et al. [30] mention in the first formal publication of the FAIR Principles: *“good data management and stewardship/shepherding is not a goal in itself, but rather a pre-condition supporting knowledge discovery and innovation”*. Papadiamantis et al. [33] identified and recommended the scientific FAIR principles to supplement the original ones and to guide data creators through the procedures that are necessary to record their data in a FAIR fashion as they are created.

As there is a clear trend of increasing demand for nanoenabled products (NEPs) with enhanced antimicrobial capacities [34] and since capacity appears to be dependent on the NMs' p-chem properties, the purpose of this study was to suggest to the research community a practical and efficient approach that enables structured data reporting using elaborated templates. We describe how variables of antimicrobial assessments are selected for FAIRification and how the data are captured. The emphasis is on preserving the most important elements that determine the antimicrobial capacity while keeping the data requirements that scientists should report to a minimum. The template enables the assessment of determinants through modeling that identifies the essential variables that permit the prediction of the NMs'/NEPs' antibacterial capacities due to the distinct combinations of NMs and applications. We explain how the developing position of data shepherd (see [33] for the definition of a shepherd) is engaged across disciplines with the objective of capturing data in a consistent and thorough manner. The reporting guidance and data template facilitate researchers and the industrial community to disclose appropriate functionality data by following the scientific FAIR principles. It also supports experts that are engaged in the data management course by displaying a pragmatic approach to template building and the curation of new data. The template can also assist with the assimilation of existing studies and the evaluation of diverse experimental environments and associated descriptors. While building the template, we did not find an alternative template to report data in a harmonized way. While several templates exist for a FAIR data capture <https://search.data.enanmapper.net/help/#dataentry> (accessed on 27 November 2021), antimicrobial assessment templates were not available.

The added element of this study in the series presented [35] is that different partners act as supplementary data creators following a chain of experimental designs that will guide the SSbD criteria. In Furxhi et al. [36], data capturing served to facilitate computational exposure models for the assessment of exposure determinants or mass flow balance models that simulate emission particle rates in occupational environments. In this case of antimicrobial capacity, the data will be used for computational purposes in an SSbD framework [37]. The requirement here is different since partners within the same project will need to reuse the data to merge safety with performance. Those cases are important since they demonstrate to the scientific community how a well-designed template can serve diverse goals, such as FAIR data capturing for the entire community, data pool creation for modeling purposes and intra-consortium partners data exchange, revealing the importance of systematic data reporting.

2. Materials and Methods

The first two published studies in the *data shepherding in nanotechnology* series [35,36] visualized the roadmap toward case-specific data-catching templates for FAIRification rationales in the ASINA project (see Figure 1) with the support from the Transnational Access program of the H2020 NanoCommons project.

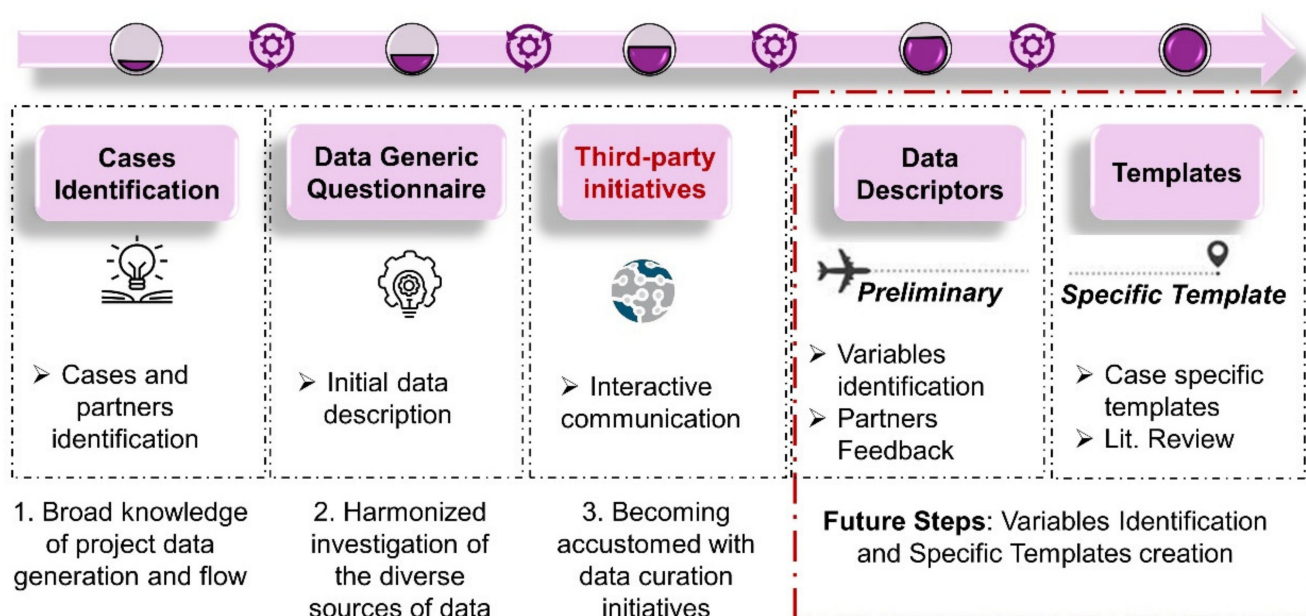


Figure 1. The path that was used for developing case-specific data capture templates for FAIRification purposes. In this study, we focused on the antimicrobial template’s final two steps (red box).

With the assistance and supervision of the data shepherd, we show the process from the recommended framework to template construction, with a focus on antimicrobial measures. The goal of the data compilation in this case was to keep track of the characterization data and the conditions of exposure and assessment for the antimicrobial study of NMs/NEPs in the ASINA supply chain [35]. The scientists (data creators) that processed and analyzed these materials were detected and a preliminary survey was circulated between the participants in order to gather information about the data to be generated (see Section 3.1). We exhibit how we moved from the preliminary questionnaires to the usage of the introductory template (see Section 3.2). We reveal the outcomes of the internal communications between partners about minimal data needs and descriptors selection, which resulted in a project consensus and the co-created template (see Section 3.3). Finally, we annotated the dataset to enhance the interoperability (see Section 3.4).

3. Results

3.1. Initial Data Description—Questionnaire

Data creators were identified and given a questionnaire to fill out in order to provide an initial description of the data to be recorded and to assist in the building of a prototype data logging template. Table 1 shows the replies of data creators regarding antimicrobial functionality measurements. The questionnaire assisted the data shepherd in organizing and directing the communication between relevant stakeholders, as well as identifying partners’ duties and anticipated outcomes. The questionnaire was established to facilitate the depiction of the data to be generated and it contained a minimal information set to begin with. The Data Management Plan (version 1) <https://www.portforward-project.eu/wp-content/uploads/2018/09/PortForward-WP9-D9.5-Data-Management-Plan-V1-Final.pdf> (accessed on 27 November 2021) of the PortForward project was sourced as inspiration for the formation of the questionnaire.

Table 1. Form for collecting initial information on each experiment from relevant partners.

Antimicrobial Capacity			
Element	Response—Data creators (STIIMA-CNR)	Response—Data creators (BioNanoPlus)	Response—Data reusers (RedOfView and CENTI)
Data Identification			
Dataset description	Antimicrobial tests on coated textiles before and after use simulation tests	Functionality analysis of nanostructured capsules that deliver active phases in cosmetics	Antimicrobial tests of cosmetic formulations
Source	Data from a measurement experiment	Data from a measurement experiment	Data from a measurement experiment
Partner's Activities and Responsibilities			
Partner owner of the data, copyright holder	The data that each partner provides to the template is under their responsibility	The data that each partner provides to the template is under their responsibility	The data that each partner provides to the template is under their responsibility
Partner in charge of data collection/analysis/storage/related WP(s)	Data collection between data creators and shepherd; construction of a measuring matrix in collaboration with stakeholders, as well as the reporting strategy throughout the project duration	Data collection between data creators and shepherd; construction of a measuring matrix in collaboration with stakeholders, as well as the reporting strategy throughout the project duration	Data creators and shepherd; bridging information for future analysis
Expected Input Variables			
Description of the information required (WPs and/or tasks) in order to move forward	- P-chem characterization of NMs deposited into the textiles	Colloidal properties (particle size, zeta potential) of NMs once integrated into the use and testing matrices	Design of the measurement matrix with contextual information to facilitate testing
Expected outcomes			
Description of the specific endpoint measurement variables/outcomes	Bacteria reduction (%): number of viable bacterial cells	Microbial log reduction	- Functionality of the coated substrate - Nanostructured capsules delivering active phases in cosmetics
Standards			
Detailed description of the methods/protocols	- AATCC100-2012—Test Method for Antimicrobial Finishes on Textile Materials - ASTM E2149-13—Standard Test Method for the Antimicrobial Activity of Agents Under Dynamic Conditions	Internal protocol involving a disc diffusion test: <i>E.coli</i> , <i>P. aeruginosa</i> and <i>S. aureus</i> are grown in Petri dishes, applying the product to be tested and then measuring the inhibition halo (zone of inhibition) obtained	- The method to evaluate the functionality of the coated substrates will depend on the type of nanomaterial to be applied on the substrate (photocatalytic, antimicrobial, etc) - The materials will be tested in agreement with the methods indicated by the nanomaterials' supplier

The responses revealed that data creators need knowledge concerning the p-chem characteristics of the NMs, such as the colloidal properties (Table 1, response from STIIMA-CNR and Bionanoplus) in order to evaluate the materials' capacity to retain antimicrobial functionality. Notice that there is no detailed explanation of which p-chem are required. The outcomes are obtained from experimental testing using various organisms and experimental standards to obtain a reduction in bacterial growth in a numeric form (percentage or log reduction). Data creators provide useful information on the protocols that will be used to extract information. On the other hand, some partners provide only limited information, such as an *internal protocol*. Data reusers will test and verify the functionality of the coated substrates before and after the implementation of the SSbD criteria with the goal to obtain the maximum functionality of NEPs while minimizing the toxicity and exposure potential. Notice that a holistic approach is taken in the ASINA case, where diverse individual testing strategies will be merged to provide the best solution (from synthesis to deposition and usage). As a result, data requirements are initially suggested but not clearly stated in

addition to the “raw” experimental data (for example, which parameters are going to be finetuned to attain the desired performance). Finally, it is important to notice that this approach, which was proposed in the SSbD concept, initially demands the deconstruction of information, which needs to be integrated into later stages, for example, the p-chem characterization, toxicological assessment and exposure potential from usage scenarios will be integrated into a single information chain. The data shepherd guides all the data creators into a consensus approach, gathering the information in advance and in such a manner that facilitates future integration and analysis. If left to the end of the project, merging the information derived from multiple partners will result in difficulties and confusion.

3.2. Preliminary Template from NIKC

Spreadsheets are a standard format that is used by most scientists in all subfields of research, and they are a decent option for data entry due to their familiarity. NanoCommons’s suggestion for data capture included the CEINT NanoInformatics Knowledge Commons (NIKC) Excel spreadsheet [38]. For information related to the template presented in Figure 2, refer to [35]. The method and measurement tabs are the focus of this study (Figure 2). When applicable, the *protocol* and *instrument* tabs (method) record knowledge about instrumentation and protocols that are linked to either sample preparation or measurement testing. The data (measurement matrix) regarding the entire experimental strategy is stored in the measurement table. The main data that are documented are the experimental conditions, information related to the NMs/NEPs and the measured outcomes, such as bacteria reduction. Finally, the *dictionary* tab contains the annotation of the descriptors. We provide the detailed metadata description of the data throughout the manuscript.

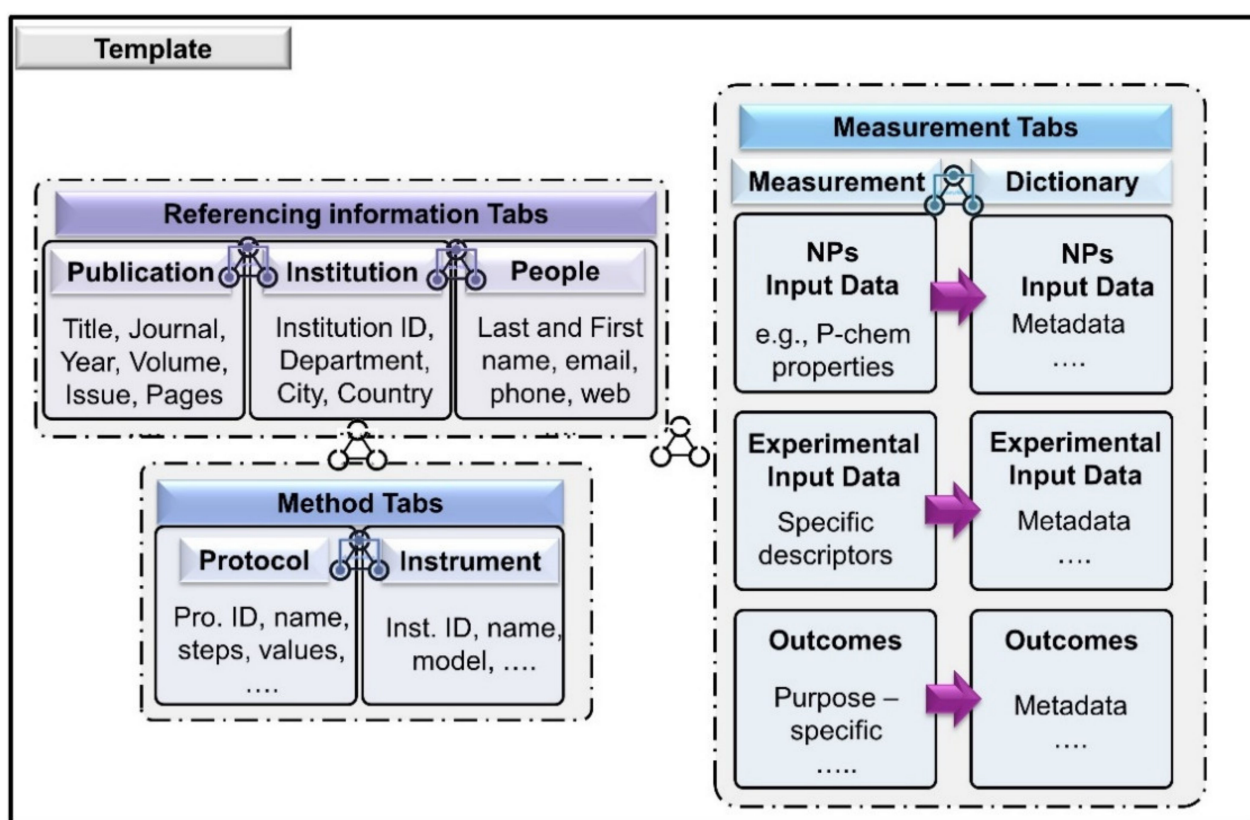


Figure 2. Visualization of the template. Each primary tab has its own set of tabs and related variables. The spreadsheet includes referencing information about data creators (people and institutions), as well as information on any publications that have used the data (publication).

3.3. Literature, Internal Communication and Descriptors Identification

In order to merge the resources, it is necessary to have the data overview from the surveys and the preliminary template on hand, as well as a literature search and numerous expert's feedback. The data shepherd and stakeholders gather knowledge of procedures and experimental settings of antimicrobial assessment and other related needed experimentations in this step, which is the most demanding element of the data management plan and FAIRification procedures.

The importance of the variables is determined by stakeholder expertise and is required to meet project objectives. Antimicrobial assessment, for example, necessitates knowledge of exposure variables, such as NM concentrations, which characterize antimicrobial capacity. Antimicrobial assessment, in combination with p-chem properties, the bacteria being exposed and the experimental conditions (including protocols and instrumentation), can provide insights into the factors that affect the antimicrobial capacity. These insights can be used to construct datasets that will enable the prediction of the antimicrobial capacity of NMs/NEPs, thus avoiding the need for excessive experimental assessments. Internal communication with expert partners within the consortium revealed that the biological interactions of NMs with bacteria or viruses were difficult to predict from the experimental data. The same NMs prepared with slight variations but the same size distribution, ion release and zeta potential resulted in different antibacterial functionality. The foregoing emphasizes the importance of preserving more data. To understand the antimicrobial determinants, which are crucial for model building, high-quality data is required. We assembled the requirements for a demo scenario of antimicrobial evaluation and the relevant stakeholders to visualize the information that is presented in the above template (Figure 3).

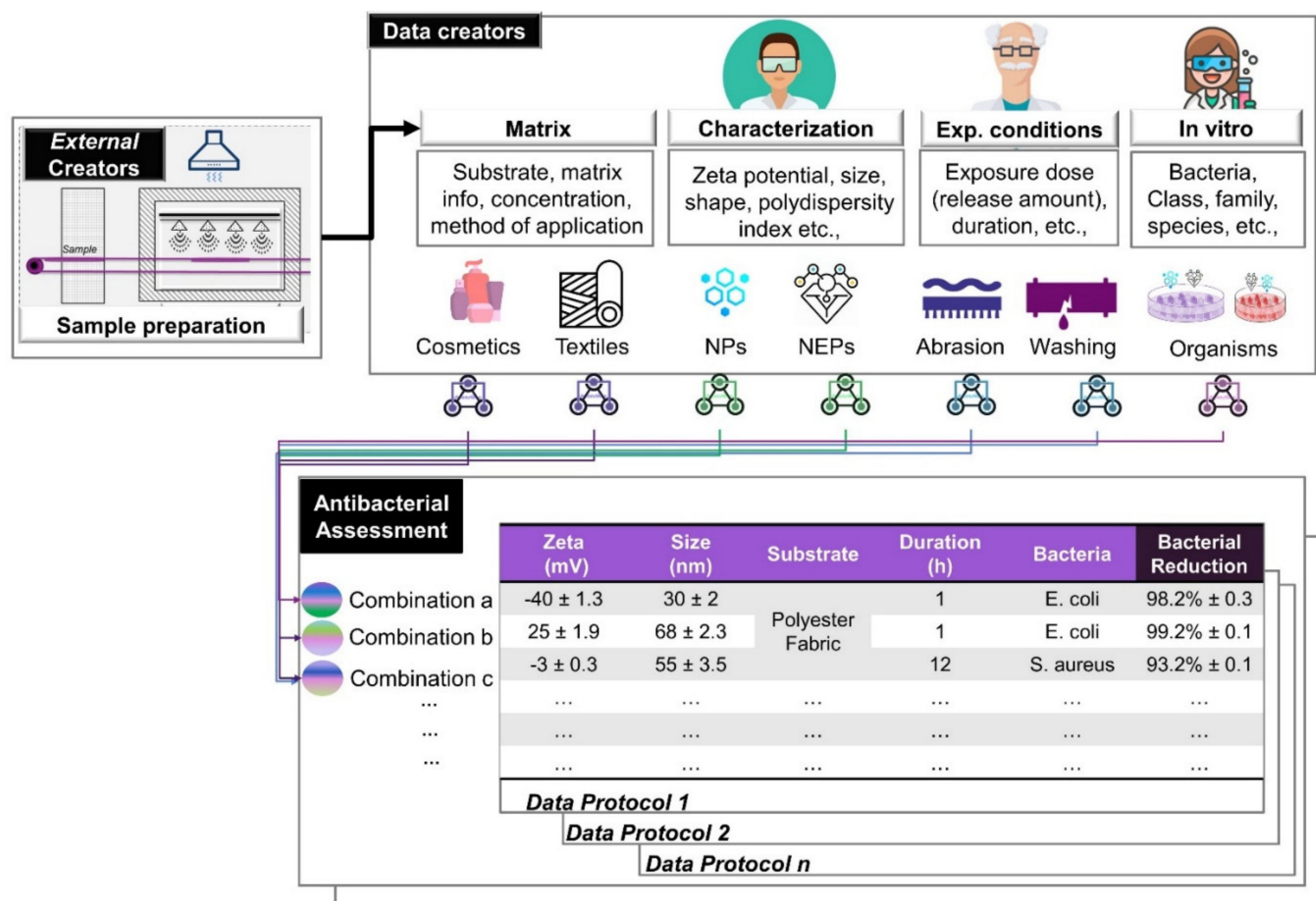


Figure 3. Visualization of antimicrobial data generation in ASINA. The figure demonstrates a snapshot of data requirements from diverse partners to ensure that antimicrobial data is useful for project goals and future reusers.

3.3.1. Nanostructured Materials Descriptors

Nanostructured materials descriptors (Table 2) contain information regarding the *testing material*, the *p-chem properties* and a description of the *sample* in which the NMs are incorporated to produce NEPs.

Table 2. Nanostructured materials descriptors that contain information regarding the material, the p-chem properties and the sample.

Category	Variables	Content	Metadata Description
Testing material	Nanomaterial (NM)	Text	NMs/nanoforms tested., ID code (ie., JRCxxx) or CAS for example. The core nanoform composition element. In the case of ASINA, a codification is used for internal communication purposes.
	Nanoenabled products (NEPs)	Text	Nanoenabled product tested. In this case, specify the NMs that were used to produce the final NEP (textiles, cosmetics, etc.) first. In the comment section, the data creator can specify whether the antibacterial testing was performed on naked NMs or NEPs.
	Provider/ manufacturer	Text	Information related to the provider of NMs/NEPs. In the case of a project, this information allows for traceability among partner information exchanges.
	Batch	Text	A code provided by a manufacturer or distributor to a manufactured material or product that is anticipated to be homogeneous after production. In the case of ASINA, the batch can reflect a sample being produced and circulated from different partners for traceability.
P-chem properties	Primary size	Number (nm) + SD	According to the EU definition, NM means a natural, incidental or manufactured material containing particles in an unbound state or as an aggregate or as agglomerate and where, for 50% or more of the particles in the number size distribution, one or more external dimensions is in the size range of 1–100 nm.
	Shape	Text	The spatial arrangement of something as being distinct from its substance. High aspect ratio NMs include nanotubes and nanowires with diverse shapes. Small aspect ratio morphologies include spherical, oval, cubic and pillar [39].
	Coating/ stabilizer	Text	Indicates the presence of a coating and/or of a stabilizer agent surrounding the particles [40]. Chemical composition of a coating layer on a material surface.
	Composition	Text and number	Chemical composition of a coating layer on a material surface. The metrics can be expressed as a percentage or a molar ratio.
	Hydrodynamic diameter	Number (nm) + SD	The diameter of a solid sphere that would exhibit the same hydrodynamic friction as the particle of interest [41]. The determined diameter is an indicator of the apparent size of the solvated particle that is approximated as being spherical.
	Polydispersity index (PDI)	Number + SD	A measurement of the size distribution, indicating the uniformity of NMs [42]. A measure of the heterogeneity of sizes of molecules or particles in a mixture.
	Zeta potential	Number (mV) + SD	The zeta potential is a measure of the electrical potential difference between the bulk fluid in which a particle is dispersed and the layer of fluid containing the oppositely charged ions that are associated with the nanoparticle's surface.

Table 2. Cont.

Category	Variables	Content	Metadata Description
	Medium tested	Number	Medium in which zeta potential was measured, e.g., water or culture.
	pH tested	Number	The pH in which the zeta potential was measured. In cases such as for cosmetics, the pH value could represent that of the final NMs solution since the sample is diluted before the zeta measurement, which results in a different pH.
	Density	Number (g/mL)	Mass (amount) of a material substance per unit volume [43].
	Viscosity	Number (cP)	The resistance of a fluid to flow when it is subjected to a force. The result is usually represented in centipoise (cP), which is equal to 1 mPa s (millipascal second).
	Ion fraction (equilibrium)	Number (wt%)	Released ion mass fraction of particles. Particles in solution exist in an equilibrium between ions and NMs. Ions released in suspension represent the synthesis conversion of ions into NMs. The higher the ion fraction, the lower the conversion. The value is expressed as a mass percent of the total testing element [44].
	Suspension concentration	Number (NM wt% $\pm$ SD)	The elemental concentration of NPs in a medium (water, cell media or biological matrix)
Sample	Application method	Text	The method of NMs deposition: dip coating, spraying, sonochemical deposition, etc.
	Substrate (matrix type)	Text	Description of the matrix (polyester fibers, cotton, polymethylmethacrylate, clay, epoxy, fil, liquid).
	Matrix	Text	Composition of the substrate, e.g., 50% X, 20% Y, 5% Z.
	Deposited concentration	Number (mg NM/g product $\pm$ SD)	Example: milligrams of active ingredient per gram of product for cosmetics; milligrams per gram of textile or grams per meter squared for textiles.

The antimicrobial activities of NMs depend on the composition, p-chem properties and surface modification [45–48]. Restricting data reporting to minimum essential data requirements, we focused on a set of p-chem properties (Table 2) rather than extensive characterization data. Previous studies revealed that properties such as the primary size [2,49], shape [50] and hydrodynamic diameter [51] play important roles in determining the antimicrobial activity of NMs [50,52–54]. The antimicrobial capacity of NMs was shown to be affected by the zeta potential, whose measurement depends on the medium tested and pH [55,56]. The inclusion of a stabilizer (or capping agent) also has a major impact on NMs' bactericidal capability [57,58]. Daly et al. [59] demonstrated the use of an ML model to discover the link between NM's p-chem characteristics, experimental conditions and bacterial viability. The study's demonstrated the effect of a coating for predicting bacterial viability. The polydispersity index (PDI) is another significant factor that affects the antimicrobial capacity, which is a metric of the particle size distribution and is indicative of the NMs uniformity [60]. Enhanced dispersibility can increase the surface area of NMs, leading to higher probabilities of interaction with the microorganisms [56] and more effective prevention of bacterial growth [61]. The ion release, as in the case of the controlled release of ions on the textile surface [62]; the density functional calculation properties (structural and electronic) directly related to NMs reactivity [63,64]; and viscosity can affect the antimicrobial properties of NMs [65,66].

As seen in Figure 3, a sample is usually circulated within the consortium to be tested for its antimicrobial capacity. Information regarding the sample, such as the application method (deposition technique) and matrix composition should be captured. There are several application methods that are used for the deposition of NMs on textiles, such as

the dip-pad technique [67,68], pad-dry-cure processes [69,70], spraying [71], grafting [72], dip coating [73], exhaustion method (immersion) [74], ultrasonic agitation and irradiation [75–77]. The finishing of the antimicrobial nanotextile can be categorized into physical and chemical groups based on the substrate/matrix (fiber) and the NM used. The physical techniques were demonstrated to be effective for the deposition of NMs on textiles, whereas, for chemical deposition, strong bonding of NMs to the fibers may considerably decrease the efficiency of the antimicrobial action of the NMs [78]. The substrates' antimicrobial capacity differs based on the matrix/composition surface [79]. For example, wool fabrics that are coated with AgNMs show higher antimicrobial activity than acrylic fabrics [80]. Some studies have shown that microorganisms adhere differently to the substrate, for example, *Staphylococcus aureus* adheres more strongly to cotton than *Escherichia coli* does [81,82]. Thus, information related to microorganisms should be reported (see Section 3.3.2). Provision of the deposited concentrations of NMs on the matrix is one of the most important elements that can make the data integrable and reusable. The concentration of the deposited NMs is commonly expressed in milligrams of nanomaterial per gram of product, where the sample is digested and the elemental concentration is measured.

3.3.2. Experimental Setup Descriptors

The observed antimicrobial activity of NMs depends on two main factors: the p-chem properties and the experimental setup conditions (Table 3).

Table 3. Experimental setup descriptors.

Category	Variables	Content	Metadata Description
Experimental conditions	Abrasion cycles	Number	Number of abrasion cycles.
	Abrasion cycles to specimen breakdown	Number	Abrasion cycles to the fabric end-of-life. A physical test for the assessment of specimen breakdown [83,84]. Specimens abraded under a test pressure using abrasive cloth for a pre-determined number of cycles or until failure occurs.
	Washing cycles	Number	Washing cycles.
Exposure conditions	Exposure dose	Number (e.g., ppm)	The dose exposed to the bacteria/microorganisms. Example: exposure dose for fabrics calculated in parts per million by considering the amount of the element on the fabrics (via ICP analysis) and the weight of fabric (1 g) per volume of inoculum (50 mL). The data creator should provide comments regarding what the dose reflects and how it was derived.
	Exposure duration	Number (h)	Either exposure duration that an in vitro system is exposed to or the incubation contact time duration, depending on the methodology.
	Culture medium	Text	Culture medium: information related to the in vitro biological system exposed.
Organisms	Initial bacterium number	Text	Initial population of bacteria.
	Class	Text	One of the bacteria classification systems comprises five kingdoms that are further split into phylum, class, order, family, genus and species. Examples of class: <i>Gammaproteobacteria</i> , <i>Sordariomycetes</i> and <i>Bacilli</i> .
	Family	Text	<i>Trichocomaceae</i> , <i>Enterobacteriaceae</i> , <i>Listeriaceae</i> , etc.
	Species	Text	<i>E. coli</i> , <i>P. aeruginosa</i> , <i>K. pneumoniae</i> , etc.

The antimicrobial properties of NEPs are strongly affected by abrasion and the detergents and water used during the washing process [85]. Prior studies have noted the

importance of the number of washing cycles on the durability and, consequently, the antimicrobial efficacy of the product [86–88]. Standard methods are required to be followed for both the abrasion and washing, with defined conditions, such as water temperature, washing speed, type of detergent and volume of the washing bath. Reporting the followed protocol allows the next users to identify additional variables of importance. Among all variables, the number of washing or abrasion cycles is the most important one that affects the outcome. The type of bacteria species in terms of their cell wall compositions (Gram-negative/positive) determines the efficacy of NMs capacity [45–48]. Gabrielyan et al. [89] showed that Fe_3O_4 NMs exhibited considerable antimicrobial activity against Gram-negative bacteria, but not Gram-positive bacteria. Therefore, it is important to report information that is associated with the type of microorganisms exposed. Exposure conditions, such as the duration that the product is in contact with the organisms (incubation time), play an important role [90]. The exposure dose and duration in in vitro systems play a critical part in the interpretation of results and should always be reported.

3.3.3. Antimicrobial Capacity

Several endpoints can be examined while performing antimicrobial testing in order to select the appropriate test system (Table 4). Various methods produce results that are generally comparable and their suitability is determined by the analytical needs [91]. The choice of the methodology that is used for testing is based on labor and financial resources [92]. A comprehensive listing of in vitro antimicrobial testing and evidence on their benefits and restrictions are described in the review study of [93].

Table 4. Measured antimicrobial capacity endpoints.

Category	Variables	Content	Metadata Description
Measured outcomes	Bacteria reduction percentage	Number (%)	Bacteria reduction is the percentage ratio of the difference between the reference bacteria concentration (e.g., inoculum, untreated sample) and the bacteria concentration after contact with the sample, and the reference bacteria concentration [94].
	Minimum inhibitory concentration (MIC)	Number ($\mu\text{g}/\text{mL}$)	The MIC is the lowest concentration of antimicrobial agent that completely inhibits the growth of the organism in tubes or microdilution wells, as detected by the unaided eye [95].
	Colony-forming unit concentration (CFU)	Number (CFU/mL)	Concentration of bacteria that can form a colony.
	Minimum bactericidal concentration (MBC) or minimum fungicidal concentration (MFC)	Number ($\mu\text{g}/\text{mL}$)	The MBC is defined as the lowest concentration of antimicrobial agent that is needed to kill 99.9% of the final inoculum after incubation for 24 h under a standardized set of conditions [93]. It is also known as the minimum lethal concentration (MLC).
	Bacteria log reduction	Number	Bacteria log reduction is defined as the common logarithm of the ratio between the bacteria concentration after contact with the sample and the reference bacteria concentration (e.g., inoculum, untreated sample).
	Zone of inhibition (ZOI)	Number (mm)	ZOI is the gap without bacteria colonies around the sample on a contaminated solid medium.
	Optical density at 600 nm (OD600)	Number (absorbance)	Optical density at a wavelength of 600 nm is used for estimating the concentration of bacteria in a liquid.
	Half maximal inhibitory concentration (IC50)	Number (molar concentration (mol/L))	IC50 is the capacity of a biocidal agent to inhibit the growth of a specific microorganism.

Several methods exist to examine and determine the antimicrobial activity of textiles [95–97]. The experimental data should be created using a single technique to provide a reliable dataset, although this is impractical. For modeling purposes, the data generated by a variety of protocols can be merged if the assay is considered. Any procedures that are applied during the assessment are described in detail in the *protocols* tab, i.e., sample preparation techniques, abrasion and washing protocols or antimicrobial assessments protocols. The template provided as Supplementary Materials includes examples that demonstrate how all the protocols are reported for p-chem data (TEM, ICP-OES, DLS and ELS), abrasion and washing stability ((ISO 105-C06, ISO 12947-2 and ISO 12947-3) and for antibacterial assessment (ASTM E2149-13). The instrumentation details are also included.

3.4. Annotation

The resulting template (measurement tab's descriptors) is semantically annotated using founded ontologies (e.g., eNanoMapper ontology, NanoParticle ontology), in compliance with the European Commission Open Data Policy and the FAIR data principles. By providing a rich metadata description of the dataset's descriptors and annotating them improves interoperability and facilitates data interpretation. Adding complete descriptions is a crucial element of enabling modeling and machine learning purposes.

4. Discussion

The template functions as a thorough spreadsheet that allows users to insert information and data on the materials examined, the experimental settings and the measured endpoints. In addition to the above information, instrumentation and protocols of the experimental strategies are captured. The template divides the data into tabs for measurements, equipment and protocols, allowing for the investigation of various antimicrobial tests, such as those performed after abrasion and/or washing cycles.

For example, in our illustration that was populated with realistic data as Supplementary Materials, the next users can identify (i) whether any publication is available and linked to the specific data generated, (ii) the institution and the personnel (and their contact details) involved in the data generation and (iii) detailed information related to the NMs/NEPs that were tested to assess their antimicrobial capacity. In detail, the reusers can extract or use data flows/rows that provide information on the p-chem properties, such as size, shape, composition, zeta potential and ion fraction. The p-chem properties are interlinked with the methodology and protocol used to generate those instances, allowing for a complete representation of the information in a transparent manner. If the protocol was applied with alterations, the steps are also reported to allow for reproducibility. In addition to the protocols, the readers can see the type and models of the instrumentation used to measure and define the p-chem properties or the desired output. On top of the p-chem data, the reader can gain information that is related to the sample/material that was tested, such as the matrix composition or the deposited concentration of NMs, which is clearly defined with its metrics (i.e., mg NM/g of product and standard deviation) and the method of application that resulted in that product (such as spray coating technology). As Supplementary Information, the experimental conditions (e.g., exposure dose and duration) of the antimicrobial testing are reported for each line, such as the abrasion cycles or the washing cycles, along with the protocol and/or instrumentation used. Finally, the desired outcome is reported (i.e., bacterial reduction, its metric (%) and how it was defined). In conclusion, the reader has a complete picture of all the information related to the testing strategy.

Heterogeneity in the formatting of data reporting impedes the evaluation, validation and/or assimilation of information. The template could be used for future review studies to collect data in a structured manner, allowing for results that are derived from different studies and or methods/protocols to be assimilated. This template also allows for future researchers to reproduce the outcomes or compare experimental settings and results, data analysts to gather information and apply modeling tools with high quality of data and data

FAIRifiers involved in databases development and maintenance to capture this ready-to-be-used information and customize it as a database instance.

The antimicrobial activities of NMs depend on the p-chem properties, composition and surface modification. Yang et al. [2] provide a summary of NMs that were tested for antimicrobial activity while showing the mean size and shape and the microorganisms (bacteria/fungi) tested. However, a review is still missing where the entire knowledge of p-chem properties and experimental conditions are summarized in order to facilitate future data extraction from studies. Computational tools can help to diminish the design space by forecasting the properties of desired NMs before synthesis, allowing for a better interpretation of their characteristics and effects while decreasing the amount of experimental trial and error.

Experiments with various methodologies are used to generate data. Standard processes should be followed while creating reliable datasets, datasets should be sufficiently large and values should be appropriate for in silico usage. There is still a long way to go to analytically address the key antibacterial properties of NMs that characterize their efficacy without a consensus on standard characterization methods, or reference microorganisms and standardized assays [23]. In addition to the standardization of methods, further harmonized outlines should be developed on how to report the p-chem properties of NMs or experimental environments and how to make these measurements analogous. The absence of metadata descriptions for experimental assays also has an impression on the transparency and, therefore, quality of the findings.

Several ongoing EU projects are focused on the SSbD notion for NMs and NEPs, for example, ASINA <https://www.asina-project.eu/> (accessed on 27 November 2021), SAbyNA <https://www.sabyna.eu/> (accessed on 27 November 2021), SABYDOMA <https://www.sabydoma.eu/> (accessed on 27 November 2021), SbD4Nano <https://www.sbd4nano.eu/> (accessed on 27 November 2021), HARMLESS <https://www.harmless-project.eu/> (accessed on 27 November 2021) and SUNSHINE <https://www.h2020sunshine.eu/> (accessed on 27 November 2021). An SSbD approach will require the knowledge of NPs'/NEPs' functionalities in order to achieve enhanced products with minimal toxicity and maximized performance/functionality. Antimicrobial testing falls into the category of functionality. The same dataset can be used to report findings that fall into a different category, such as anti-aging or antioxidant capacities, by simply inserting a column into the spreadsheet, allowing one template to capture diverse information around the functionality aspect of NMs or NEPs. According to the minimum requirement principle of FAIRness, we have restricted the p-chem properties to those (by consensus) that are the most important to the outcome. For example, in the case of cosmetic NEPs, density and viscosity should be reported, along with the anti-aging capacity. This means there may be features in the template that are not relevant to other outcomes, for example, the abrasion or washing cycles are applicable only in the case of textiles durability and antimicrobial retention capacity. The template can be useful in projects around the SSbD aspect by allowing the data creators to report the data in a systematic way, ultimately allowing for the integration of knowledge that was derived from different projects.

As per the FAIR principles, the metadata description and annotation element promote interoperability and reusability by explaining the framework in which the data were acquired. Simultaneously, adequate metadata permits reusers to determine whether they can utilize the data in contexts other than those for which it was originally aimed [33]. In order to do so, we used several ontological IDs from diverse libraries (such as eNanoMapper <https://biportal.bioontology.org/ontologies/ENM> (accessed on 27 November 2021) and NanoParticle Ontology <https://biportal.bioontology.org/ontologies/NPO> (accessed on 27 November 2021)). Jeliaskova et al. [18] presented an overview of the eNanoMapper database, as well as the data it contains and the approach, suggestions and challenges to FAIRifying data. The authors emphasize the deficiency of reusable, organized data, as well as the necessity for simple and straightforward reporting formats, metadata explanations, ontologies and standardized nomenclature. The authors acknowledged that

the data given at the moment is insufficient for computational objectives. This template's terminology, metadata description and the inclusion of the experimental protocol and settings can help the community's effort toward the FAIR goal. The eNanoMapper database provides a FAIR-aligned Nanosafety Data Interface <https://search.data.enanomapper.net/> (accessed on 27 November 2021), with a search application to discover data across database instances [18]. Among the diverse data that are available, we did not find any dataset containing antimicrobial capacity data, signifying the importance of initiating the capturing of these data in a systematic way. For the moment, antimicrobial data is not yet in a format that is suitable for reusable purposes (available only scattered in literature), and tremendous efforts are needed to be put into extracting data (Mirzaei et al. [23]).

From the standpoint of a data shepherd, the most difficult element was transitioning from the questionnaire's defined and summarized information to the comprehensive condition of a data entry template. Data creators, for example, were required to deliver information regarding the p-chem characteristics of the NMs based on their responses to the questionnaire. However, from the initial questionnaire that was distributed among the partners, ambiguity around which p-chem properties to report was evident. Internal communication between the partners provides clarity and helps to reach a consensus among partners regarding project goals. For instance, one partner suggested that the amount released under use and testing conditions is needed in order to demonstrate a material's capacity to retain antimicrobial functionality. However, after the internal calls, a consensus on alternatives was reached and such information was not required to be reported/tested by different partners. Details like this reveal the communication importance among the stakeholders, which is often underestimated in large consortia. Some partners provided only information as an *internal protocol*. The role of the data shepherd in this case, for example, is to disclose the information of the protocol and make the data reusable and transparent.

In ASINA, data shepherds consider their data responsibility as a stream of efforts by data creators and partners. Dedicated data-capturing calls are performed periodically with all the stakeholders, where data requirements and data logging into templates are discussed. This improves the data consistency and quality while ensuring improved communication. This also streamlines data collecting procedures and ensures that the data is directly applicable to reusers. The connection between the data shepherd and the data creators is crucial to the reliability, quality and application of the data generation and capturing strategy [33].

Because contextual information and metadata are often lacking, reproducing comprehensive measurements might be difficult. Communication is frequently overlooked as being less crucial than conducting scientific experiments. The main obligations for the data shepherd are expediting communication and awareness between the stakeholders of the data to be captured while constantly emphasizing the necessity of metadata reporting. Data FAIRness represents a challenge for the scientific experimental data and, most importantly, a mental shift of the scientific community toward data reporting. Data shepherding's innovative role is emerging [33]. The shepherd does not disturb the experimental design; instead, they facilitate information flow and assure appropriate data and metadata gathering. The ability to communicate each stakeholder's needs in a clear and thorough manner is critical to this responsibility. The shepherd is a devoted role in several fields that should not be reflected as a negligible calling, as it is responsible for the project data synopsis, communication administration, case-specific data template creations, data FAIRification and ensuring the mental shift of the community toward FAIR data. Data shepherding for a multi-partner scientific research collaboration necessitates separate procedures and resources.

5. Conclusions

Functionality data are the cornerstone data as they precede health- and environmental-related data; they quantitatively comprise the reason safety is even considered. In this paper,

we demonstrate the data shepherd template creation workflow and its related steps. We provide the template for experimentalists primarily to report findings in a FAIR way and secondarily for the nanocommunity to enrich material behavioral insights and accelerate innovation.

Supplementary Materials: The following are available online at <https://www.mdpi.com/article/10.3390/coatings11121486/s1>, Data template.

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