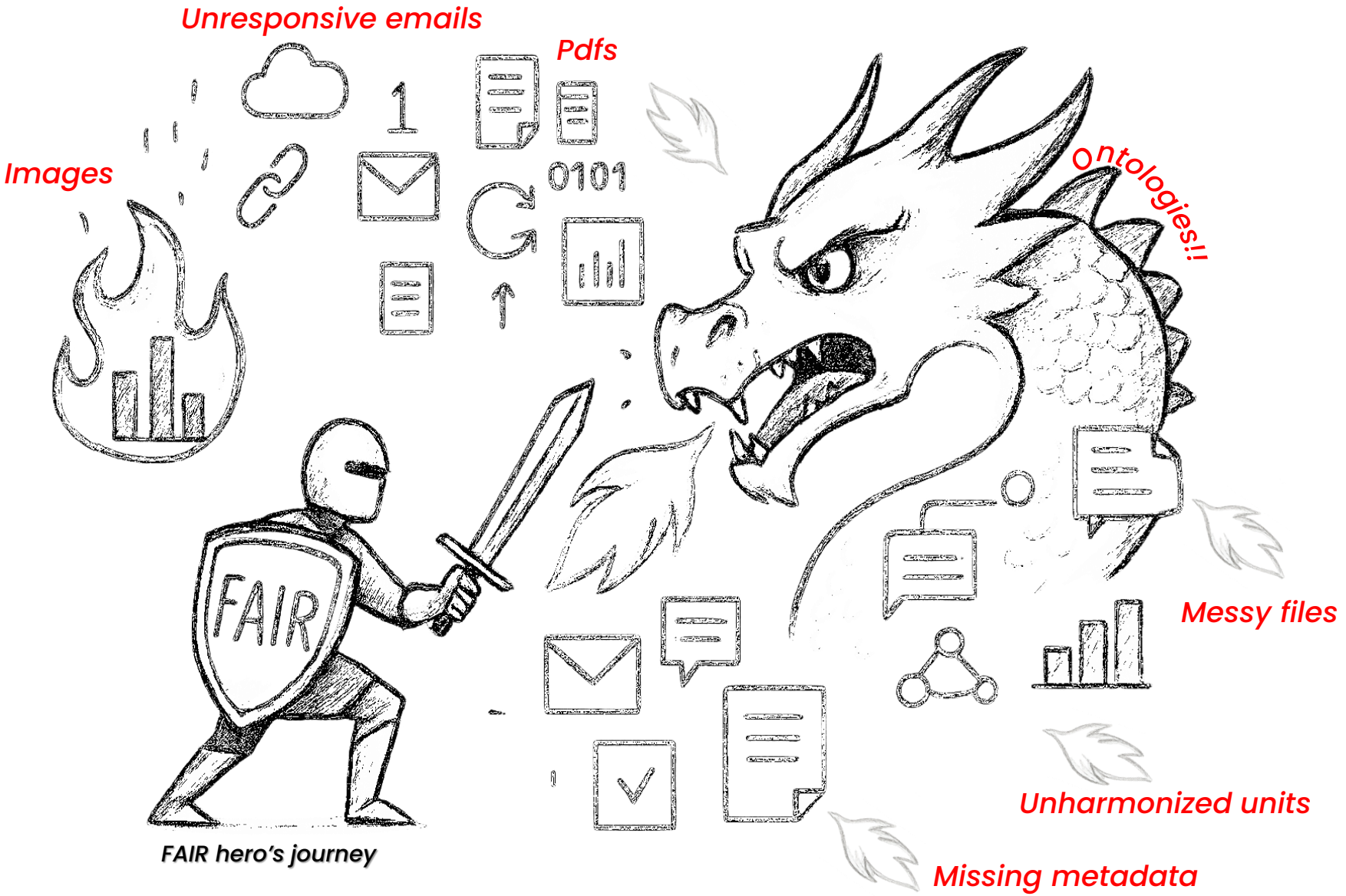
FAIR Data in SSbD

Irini Furxhi
ISSMC-CNR, Faenza, Italy

FAIR hero's journey

Funded by the European Union



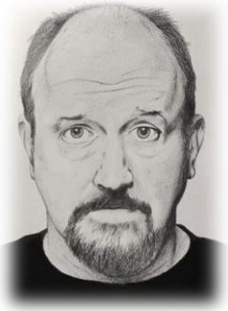
Fighting Dragons

Funded by the European Union

The Prophecy

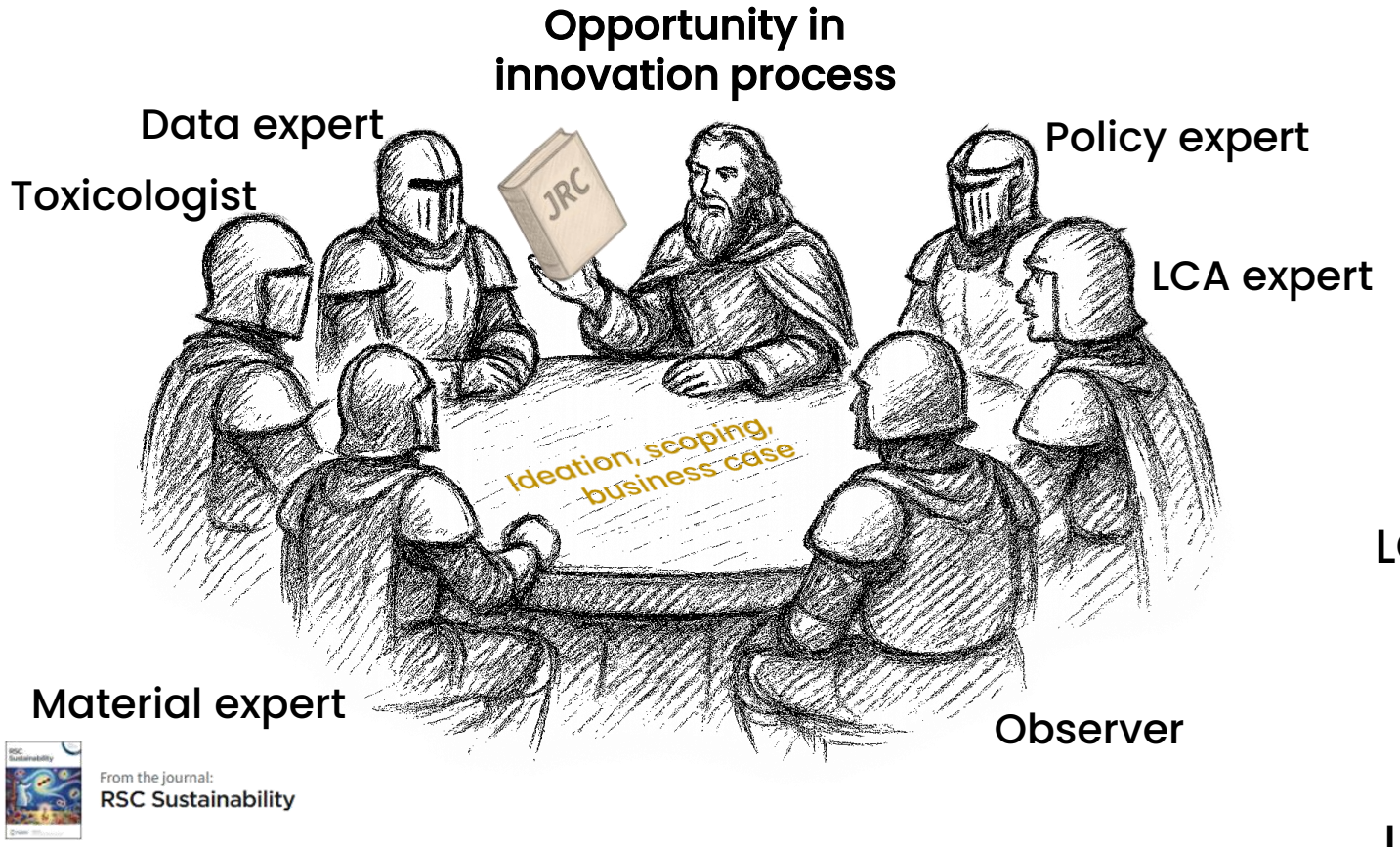
"In the dark ages of data, an ancient rune was carved with four commands..."

But, it's easier to write runes than to live by them...



"I have a lot of beliefs, and I live by none of them."
— Louis C.K.

Funded by the European Union



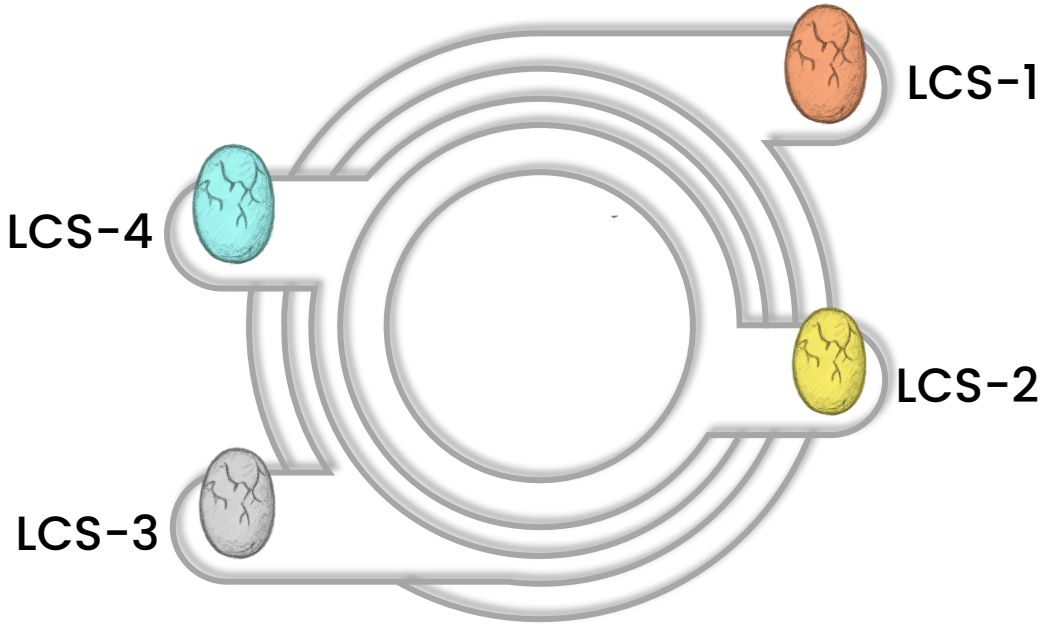
From the journal:
RSC Sustainability

The FAIR principles as a key enabler to operationalize safe and sustainable by design approaches

Check for updates

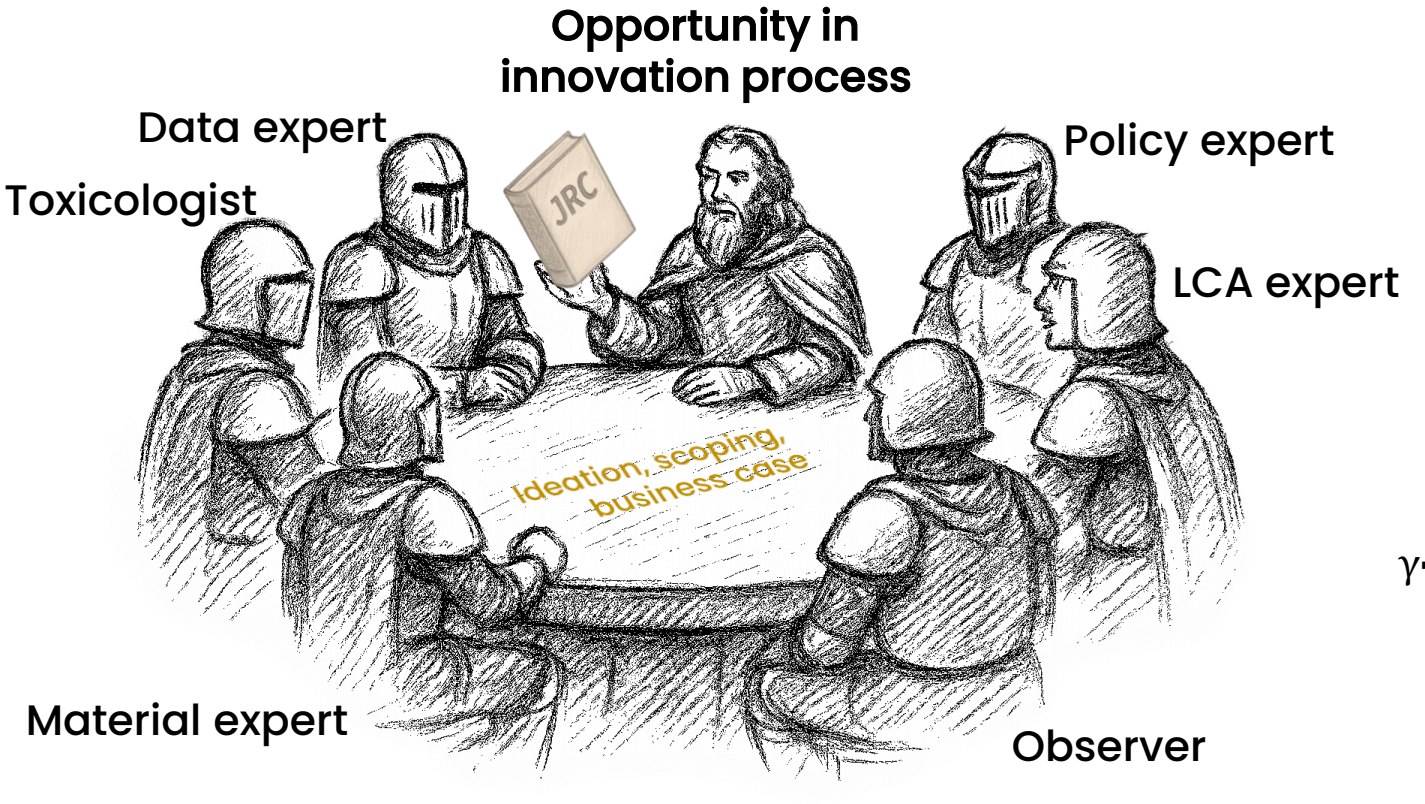
Achilleas Karakoltzidis, Chiara Laura Battistelli, Cecilia Bossa, Evert A. Bouman, Irantzu Garmendia Aguirre, Ivo Iavicoli, Maryam Zare Jeddi, Spyros Karakitsios, Veruscka Leso, Magnus Løfstedt, Barbara Magagna, Denis Sarigiannis, Erik Schultes, Lya G. Soeteman-Hernández, Vrishali Subramanian and Penny Nymark

SSbD Journey Begins

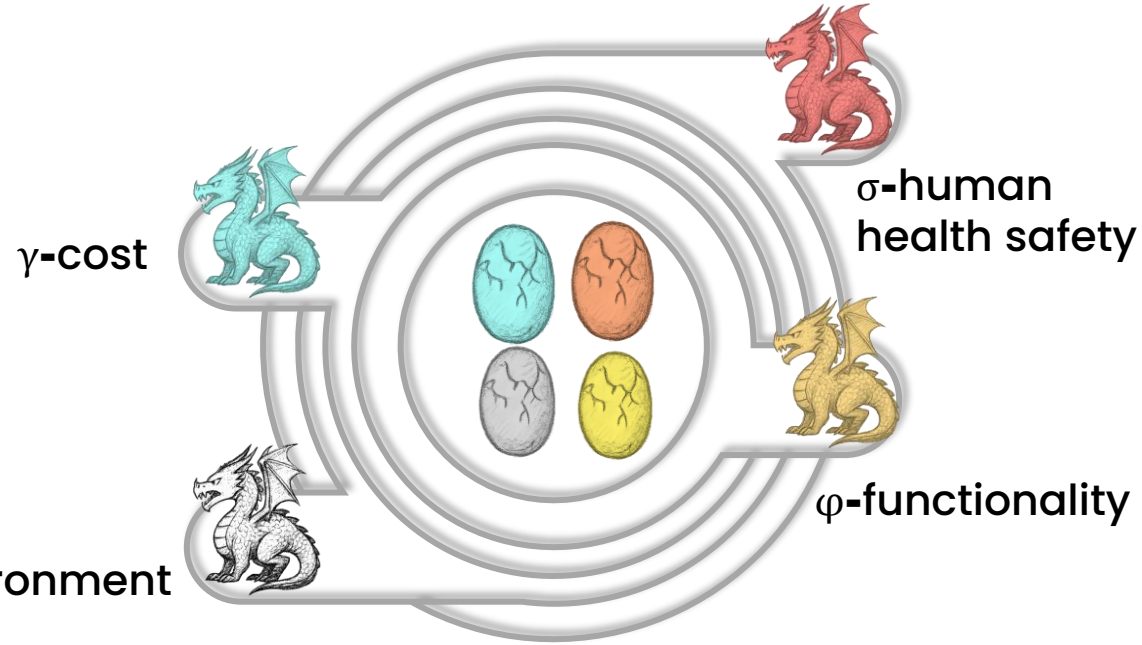


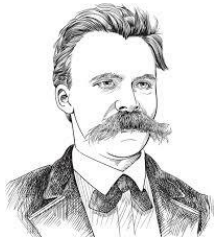
FAIR dragons lurk at every life cycle stage…

Funded by the European Union



SSbD Journey continues





"if you gaze long into an abyss, the abyss also gazes back to you."
-Nietzsche

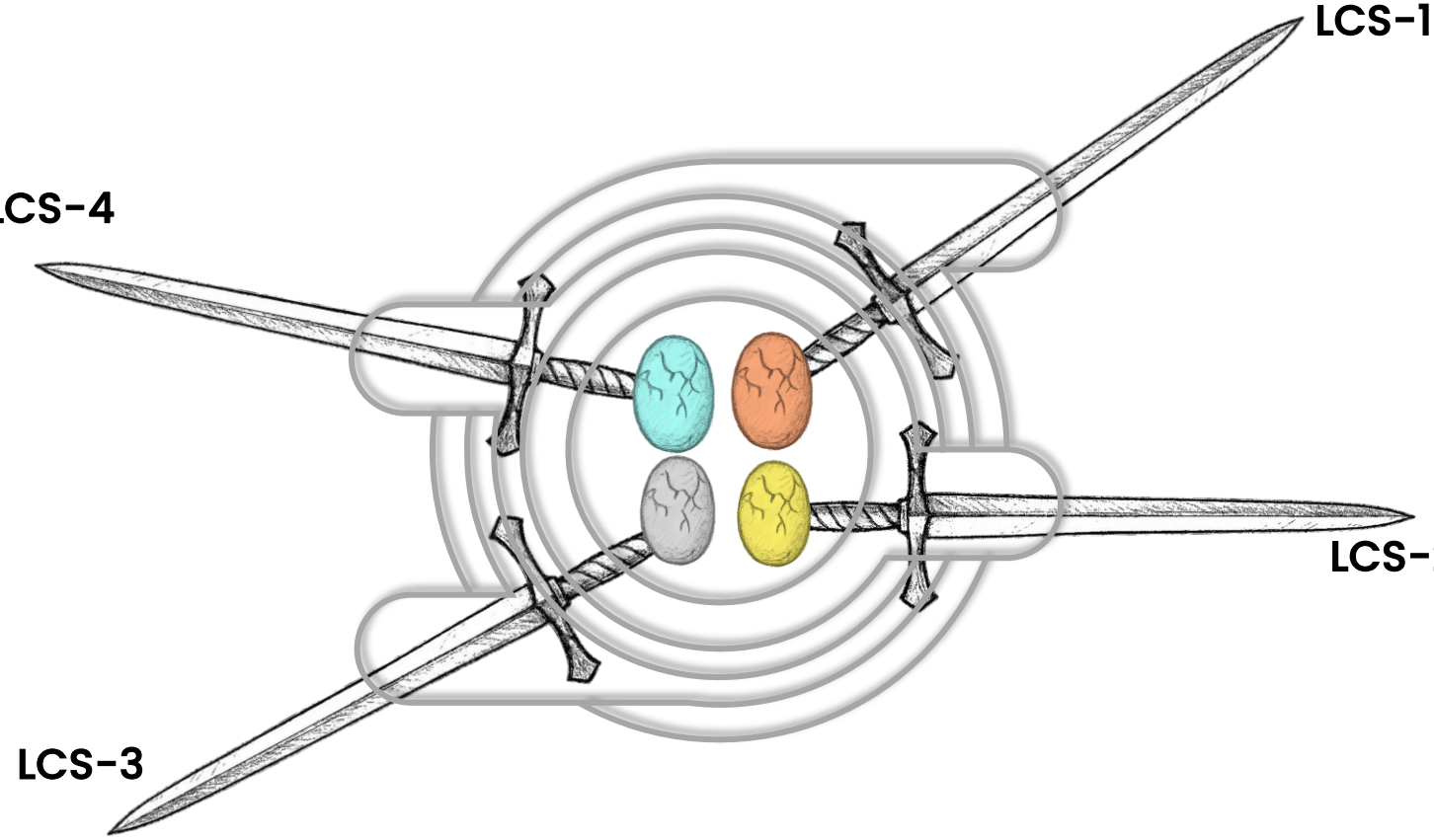
FAIR dragons lurk at every dimension …

Funded by the European Union

SSbD data - Begins

σ-human health safety
ε-environment
ϕ-functionality
γ-cost

LCS-4



LCS-1

σ-human health safety
ε-environment
ϕ-functionality
γ-cost

LCS-2

σ-human health safety
ε-environment
ϕ-functionality
γ-cost

σ-human health safety
ε-environment
ϕ-functionality
γ-cost

LCS-3

FAIR dragons lurk at every dataset ...

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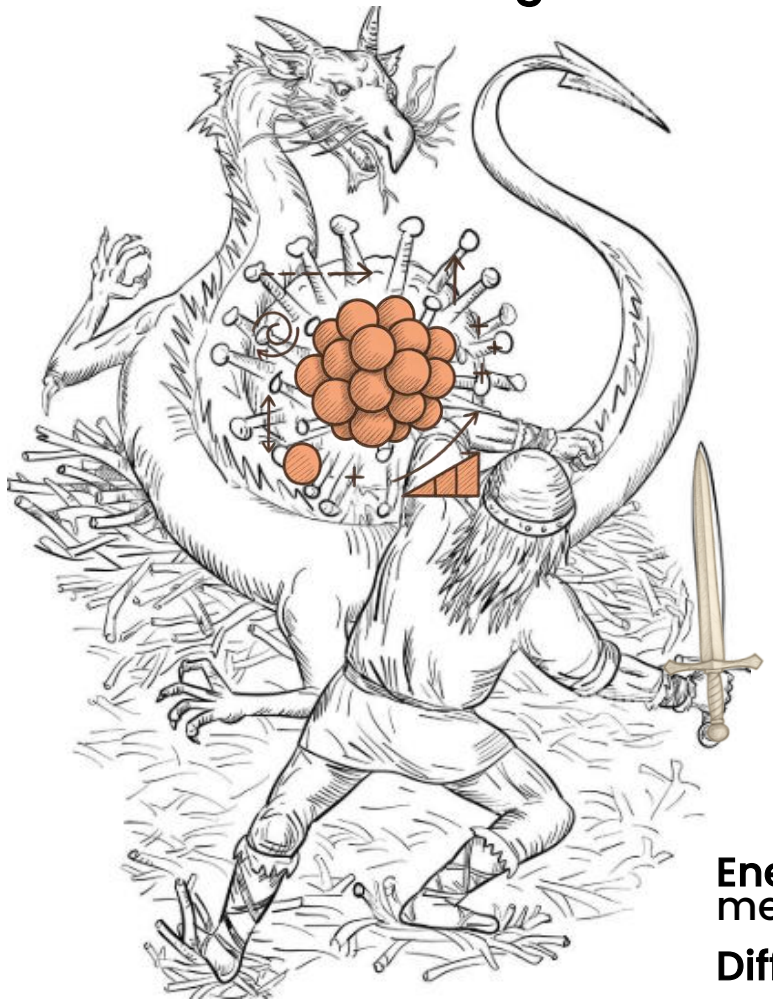
The Forge of Synthesis

Particles are born but their origins are forgotten...



Enemy: The metadata eater

Difficulty: 7/10

THE PROCESS

R potion (R1)

-Precursors (CAS, purity, supplier) & concentrations

-Synthesis method (step-by-step protocol)

-pH / Temperature /duration of reaction solutions

-Stabilizing agents & concentrations

-Instrument settings (temperature, pH, time, pressure)

-Batch number + replicates

- Use of external fields (electric, magnetic, ultrasound)

-Yield (%), scale of process

INFORMATION ON NANOMATERIALS

R potion (R1.3)

- Chemical Composition
- Density
- Particle size & distribution
- Aspect ratio/shape
- Surface chemistry
- Specific surface area
- Isoelectric point
- Dissolution (rate)
- Possible contaminants/impurities

Funded by the European Union

F potion

(F2)

TREATMENT PRIOR TO TESTING

- Treatment (e.g. warming, grinding)
- Preliminary purification step (if any)
- Final concentration
- Final preparation of a solid

STABILITY AND STORAGE CONDITIONS

- Storage condition
- Homogeneity under test conditions and storage
- Stability in the medium
- Solubility and stability in the solvent/vehicle
- Reactivity of the test material

R potion

(R1.3)

MINIMUM AMOUNT OF METADATA

-Biological and Biomedical Investigations (MIBBI)

-Bio–nano Experimental Literature (MIRIBEL)

-Nanomaterial Biocorona Experiments (MINBE)

-Simulation Experiment (MIASE)

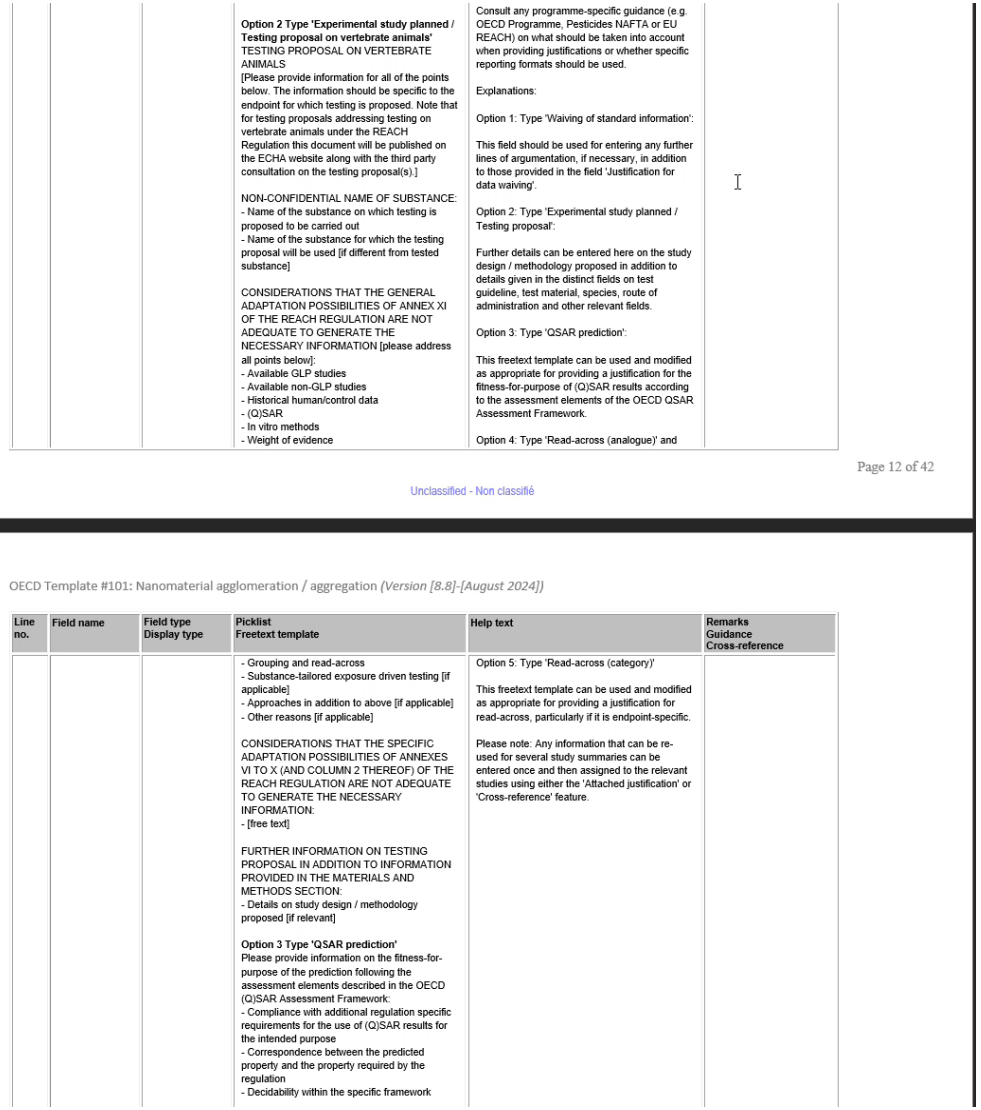
-Annotation of Models (MIRIAM)

eNanoMapper Template Designer

Designing data entry templates for eNanoMapper

The Template Designer App is under development right now

KC, JRC, GRACIOUS



Line no.	Field name	Field type Display type	Picklist Freetext template	Help text	Remarks Guidance Cross-reference
			Option 2 Type 'Experimental study planned / Testing proposal on vertebrate animals' TESTING PROPOSAL ON VERTEBRATE ANIMALS [Please provide information for all of the points below. The information should be specific to the endpoint for which testing is proposed. Note that for testing proposals addressing testing on vertebrate animals under the REACH Regulation this document will be published on the ECHA website along with the third party consultation on the testing proposal(s).] NON-CONFIDENTIAL NAME OF SUBSTANCE: - Name of the substance on which testing is proposed to be carried out - Name of the substance for which the testing proposal will be used [if different from tested substance] CONSIDERATIONS THAT THE GENERAL ADAPTATION POSSIBILITIES OF ANNEX XI OF THE REACH REGULATION ARE NOT ADEQUATE TO GENERATE THE NECESSARY INFORMATION [please address all points below]: - Available GLP studies - Available non-GLP studies - Historical human/control data - (Q)SAR - In vitro methods - Weight of evidence	Consult any programme-specific guidance (e.g. OECD Programme, Pesticides NAFTA or EU REACH) on what should be taken into account when providing justifications or whether specific reporting formats should be used. Explanations: Option 1: Type 'Waiving of standard information': This field should be used for entering any further lines of argumentation, if necessary, in addition to those provided in the field 'Justification for data waiving'. Option 2: Type 'Experimental study planned / Testing proposal': Further details can be entered here on the study design / methodology proposed in addition to details given in the distinct fields on test guideline, test material, species, route of administration and other relevant fields. Option 3: Type 'QSAR prediction': This freetext template can be used and modified as appropriate for providing a justification for the fitness-for-purpose of (Q)SAR results according to the assessment elements of the OECD QSAR Assessment Framework. Option 4: Type 'Read-across (analogue)' and	

Page 12 of 42

Unclassified - Non classifié

OECD Template #101: Nanomaterial agglomeration / aggregation *(Version [8.8]-[August 2024])*

Line no.	Field name	Field type Display type	Picklist Freetext template	Help text	Remarks Guidance Cross-reference
			- Grouping and read-across - Substance-tailored exposure driven testing [if applicable] - Approaches in addition to above [if applicable] - Other reasons [if applicable] CONSIDERATIONS THAT THE SPECIFIC ADAPTATION POSSIBILITIES OF ANNEXES VI TO X (AND COLUMN 2 THEREOF) OF THE REACH REGULATION ARE NOT ADEQUATE TO GENERATE THE NECESSARY INFORMATION: - [free text] FURTHER INFORMATION ON TESTING PROPOSAL IN ADDITION TO INFORMATION PROVIDED IN THE MATERIALS AND METHODS SECTION: - Details on study design / methodology proposed [if relevant] **Option 3 Type 'QSAR prediction'** Please provide information on the fitness-for-purpose of the prediction following the assessment elements described in the OECD (Q)SAR Assessment Framework: - Compliance with additional regulation specific requirements for the use of (Q)SAR results for the intended purpose - Correspondence between the predicted property and the property required by the regulation - Decidability within the specific framework	Option 5: Type 'Read-across (category)' This freetext template can be used and modified as appropriate for providing a justification for read-across, particularly if it is endpoint-specific. Please note: Any information that can be re-used for several study summaries can be entered once and then assigned to the relevant studies using either the 'Attached justification' or 'Cross-reference' feature.	

42 pages: TG110 Template #101: Nanomaterial agglomeration / aggregation (Version [8.8]-[August 2024])

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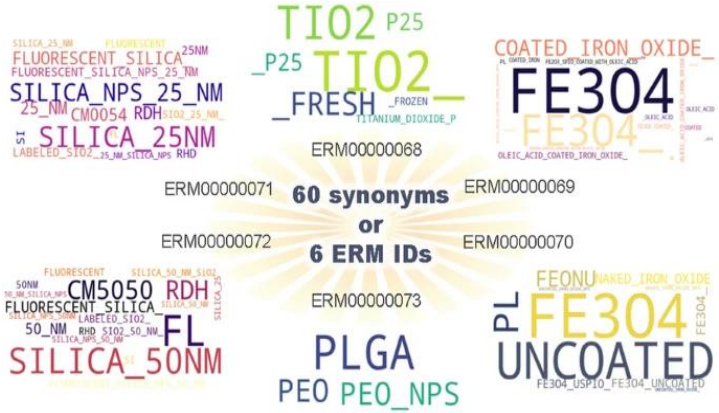
The Forge of Synthesis

Particles are born but their origins are forgotten...

F potion (F1)

CAS Number	13463-67-7
InChI	1S/O2Ti/c1-3-2
SMILES	O=[Ti]=O
PubChem CID	26042
EC Number	236-675-5

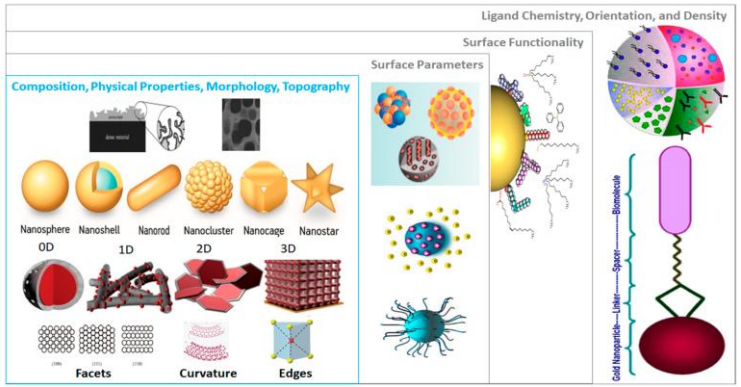
ERM Identifier



ERM00000068-ERM00000073

*van Rijn, J., et al. . J Cheminform **14**, 57 (2022). https://doi.org/10.1186/s13321-022-00614-7*

Nano InChI



NinChI=0.00.1A/Au/msh/s2t-9!/O2Si/c1-3-2/msp/s20d-9/k000/y2&1

*Lynch, I.; et al. Nanomaterials **2020**, 10, 2493. https://doi.org/10.3390/nano10122493*

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The Forge of Synthesis

Particles are born but their origins are forgotten...

F potion

(F3, F4)

A1.1

A potion

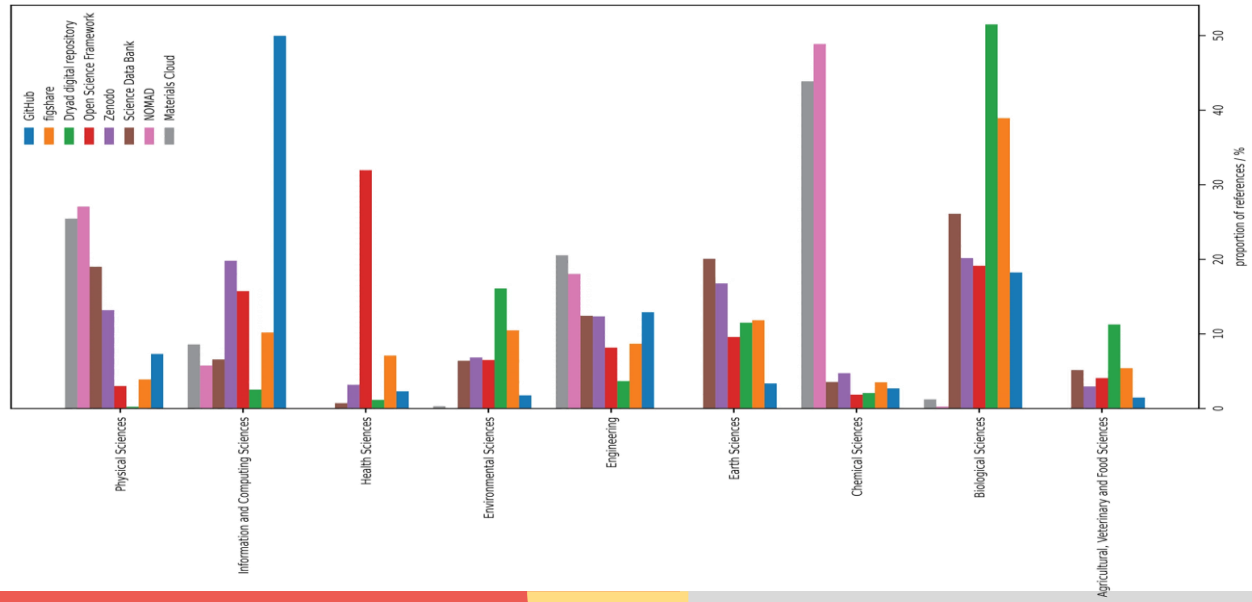
(A1, A1.1, A1.2, A2)

R potion

(R1.1)

Repositories
Zenodo
Figshare
Dryad
Science bank
NOMAD
Materials cloud
caNanoLab
eNanoMapper

Persistent ID	Assign a DOI
Metadata file	who, what, when, how
License	CC-BY, CC0,
Access	HTTP, SPARQL, FTP
Format	Machine-readable formats **or lest Excel**



https://www.nature.com/articles/s42004-024-01143-0/figures/2

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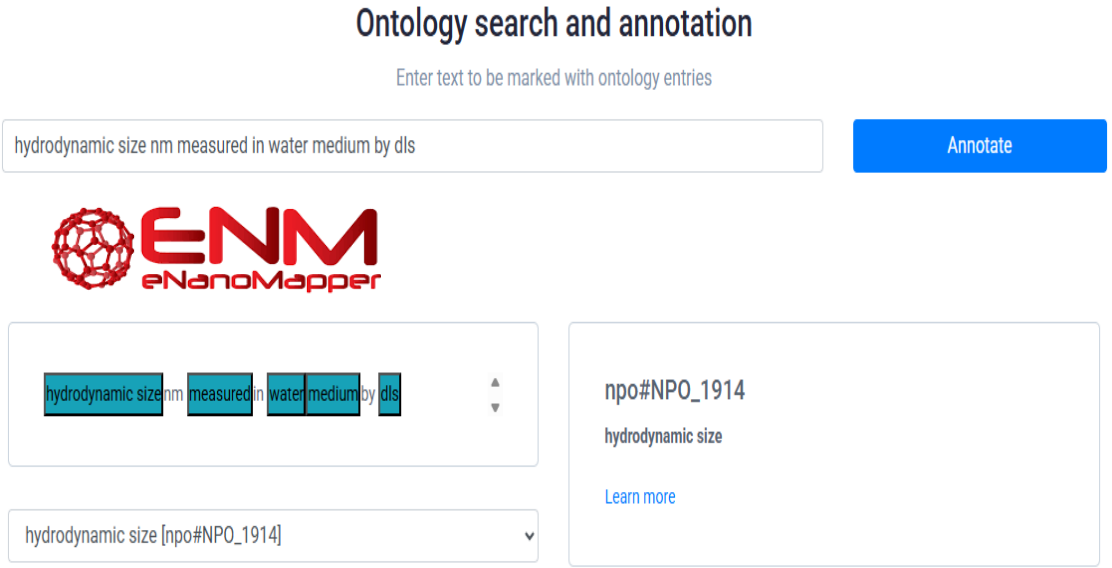
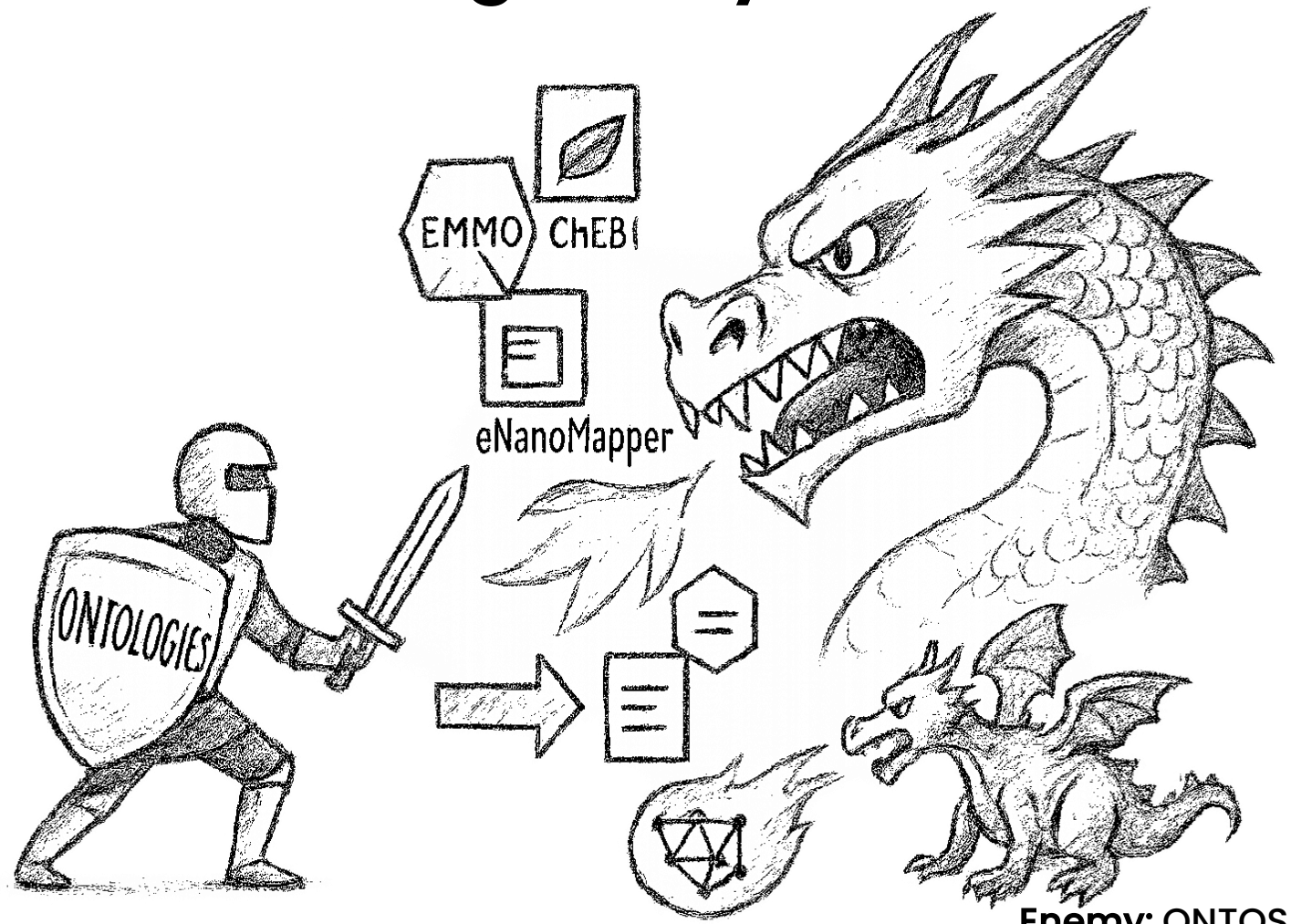
The Forge of Synthesis

I potion (I1, I2)

Nanomaterials & coatings	eNanoMapper, MATERIALSMINE
Chemical reagents	ChEBI
Synthesis methods / processes	EMMO
Biological experiments	OBI
Bioassay outputs	BAO
Environmental conditions	ENVO
Physical properties	PATO + UO





Enemy: ONTOS

Difficulty: 7/10

De Baas et al., "Review and Alignment of Domain-Level Ontologies for Materials Science," in IEEE Access, vol. 11, pp. 120372-120401, 2023, doi: 10.1109/ACCESS.2023.3327725.

Aameri B, Poveda-Villalón M, Sanfilippo EM, et al. The materials design ontology. Semantic Web. 2023;15(2):481-515. doi:10.3233/SW-233340

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Digital Twins / Industrial IoT

B2MML is an XML/JSON known as IEC/ISO 62264.
A standard way to exchange data between business and manufacturing systems

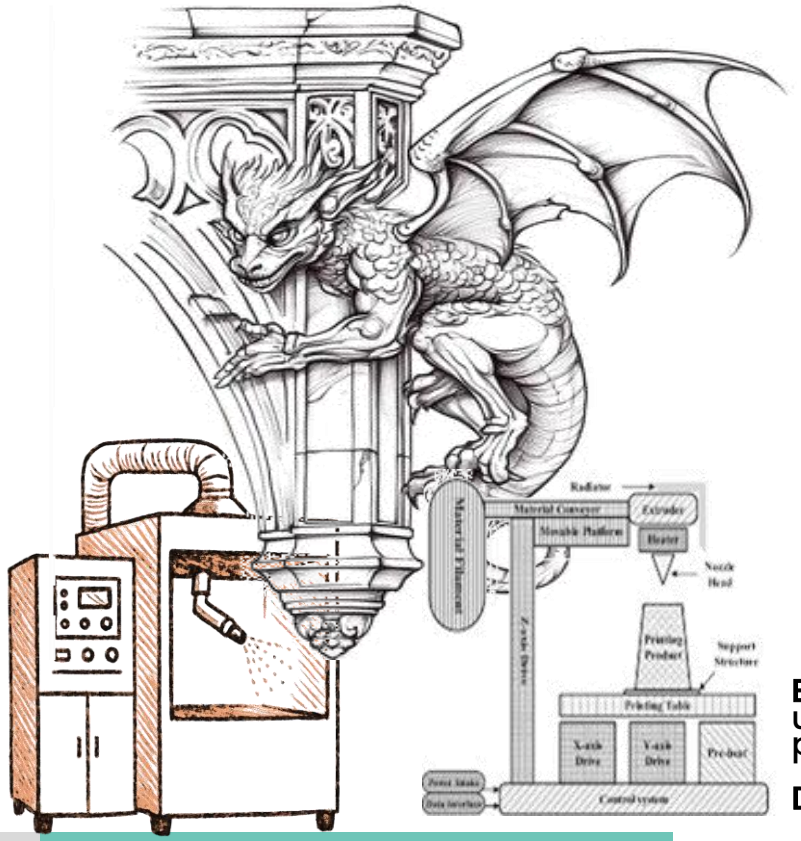
THE PROCESS ITSELF

- **A text description** (name, ID, machine function, operating mode, control system)
- All **process parameters** (steps number, input materials, units, duration, temperature, flow rate, distance to substrate)
- Graphs and pictures
- Version of standard operating procedure (SOP)
- Calibration logs, Ambient information
- Software versions
- Year, location

R potion

The Factory of Forgotten Fields

“Great machines roar, but no one writes down their secrets…”



Enemy: “The unknown process”

Difficulty: 10/10

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THE PROCESS IN ACTION

R potion

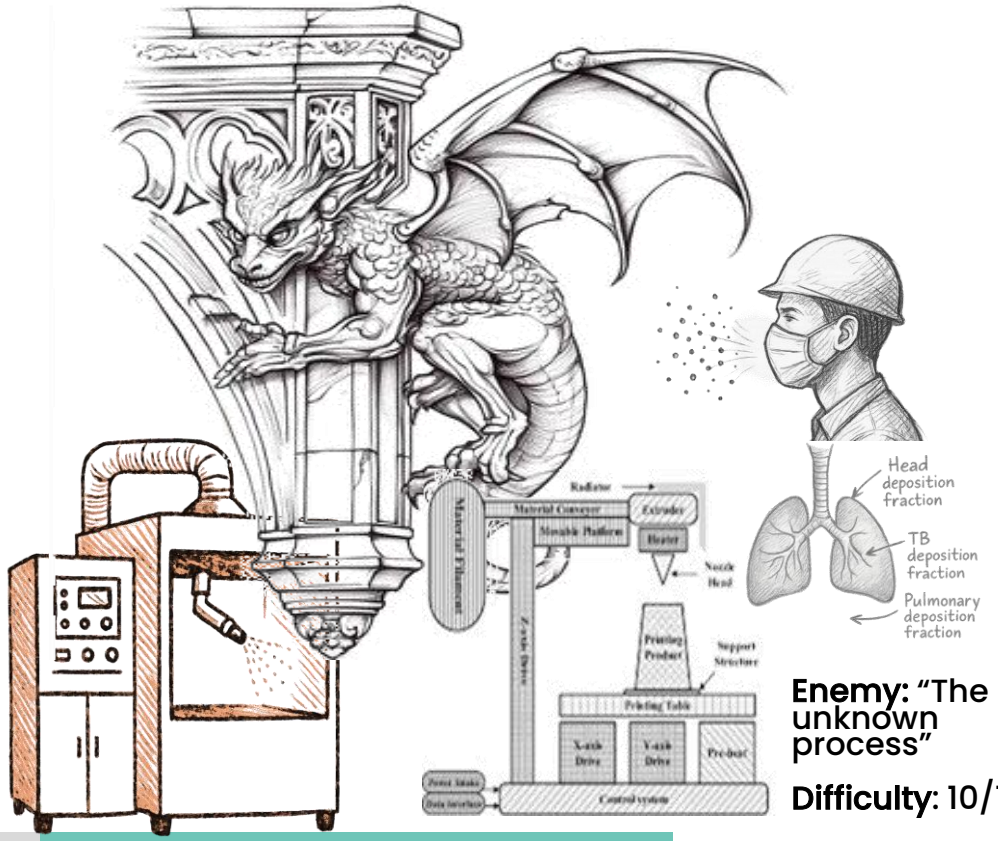
-**Aerosol measurements:** number conc. (e.g., SMPS, OPC), size distribution, Mass conc. (Teflon + ICP-MS)
-**Background levels**: before and after process
-Location of measurement
-Duration of process / sampling rates
-Instrumentation & calibration processes
-**Sampling details**

Raw data - time series format

Simulated data - for example MPPD/ TEAS/ NAMs/LCA
Record software data / input - outputs and assumption

The Factory of Forgotten Fields

"Great machines roar, but no one writes down their secrets..."



Enemy: "The unknown process"

Difficulty: 10/10

Sapel, P et al. (2024). https://doi.org/10.1007/s10845-024-02425-z
https://zenodo.org/records/4665253#.YOlza-hKguU
https://www.mdpi.com/2079-4991/11/7/1818#B15-nanomaterials-11-01818

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A template example.

Contributing scenario: Task 1

Nano Object Descr.

NO, Matrix, State, concentration of NO, etc.,

93 wt.% Cu

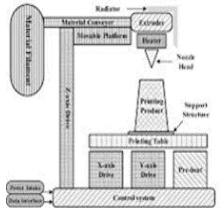
Emission Control

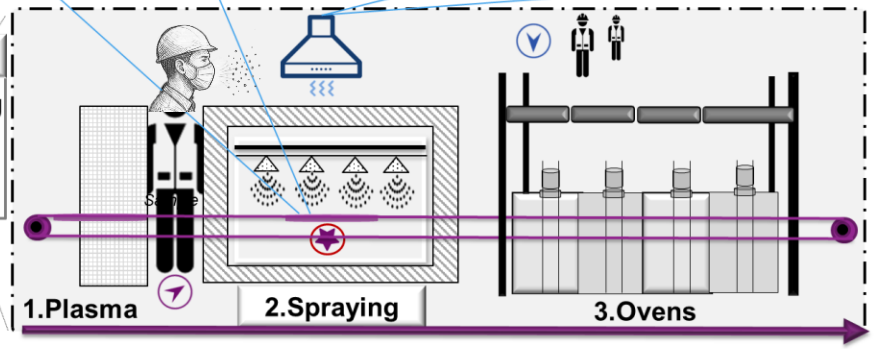
Control Efficiency, LEV flow rate, random air flow etc.,

56 m³/min

Process Descr.

Emission rates, handling rates, production rates, Speed, pressure, temp., nozzles number etc.,





- Near Field
- Far Field
- Source

Env. Descriptors

Room size, ventilation, etc.,

On-line Measurement data

09:32-10:08	560.2 (cm³)	6238.8 (cm³)	435.8 (cm³)
10:18-10:52	760.4 (cm³)	7519.5 (cm³)	376.1 (cm³)
...	...	...	...

	Pre-process	During	Post
09:32-10:08	262.8 (cm³)	550.3 (cm³)	292.1 (cm³)
...	...	...	...

Data OPC Instrument

Data SMPS Instrument

Data DustTrack Instrument

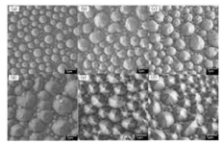
Off line Measurement data

09:25-12:45	120 (µg /m³)	1217 (µg /m³)
...	...	...

e.g., for Near Field

Background

Date	24 (µg m³)



Nano p-chem info SEM

Data Gravimetric filters

Furxhi, I.; *Nanomaterials* **2021**, *11*, 1818. https://doi.org/10.3390/nano11071818

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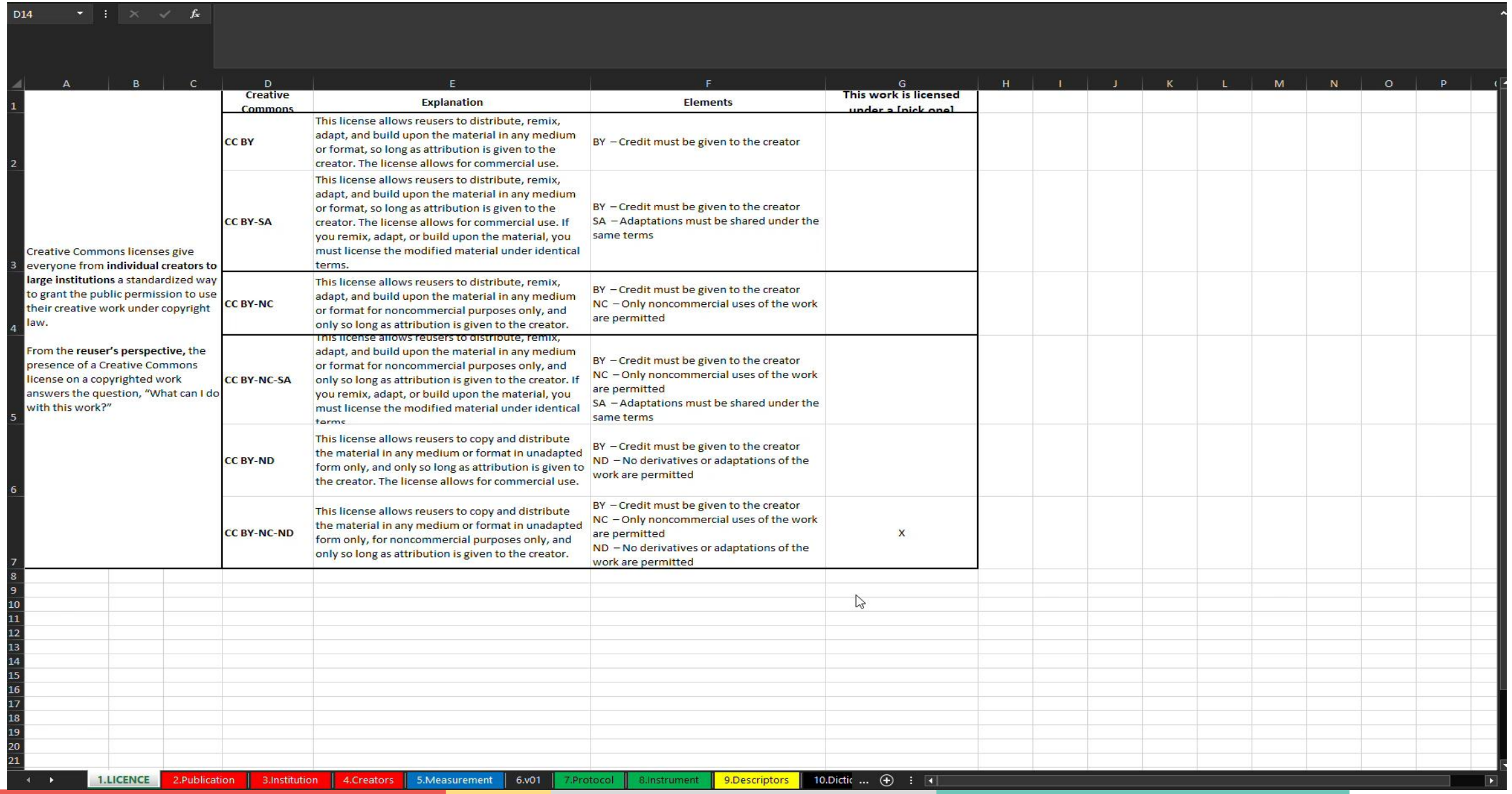

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CC BY-SA	This license allows reusers to distribute, remix, adapt, and build upon the material in any medium or format, so long as attribution is given to the creator. The license allows for commercial use. If you remix, adapt, or build upon the material, you must license the modified material under identical terms.	BY – Credit must be given to the creator SA – Adaptations must be shared under the same terms	
CC BY-NC	This license allows reusers to distribute, remix, adapt, and build upon the material in any medium or format for noncommercial purposes only, and only so long as attribution is given to the creator.	BY – Credit must be given to the creator NC – Only noncommercial uses of the work are permitted	
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CC BY-ND	This license allows reusers to copy and distribute the material in any medium or format in unadapted form only, and only so long as attribution is given to the creator. The license allows for commercial use.	BY – Credit must be given to the creator ND – No derivatives or adaptations of the work are permitted	
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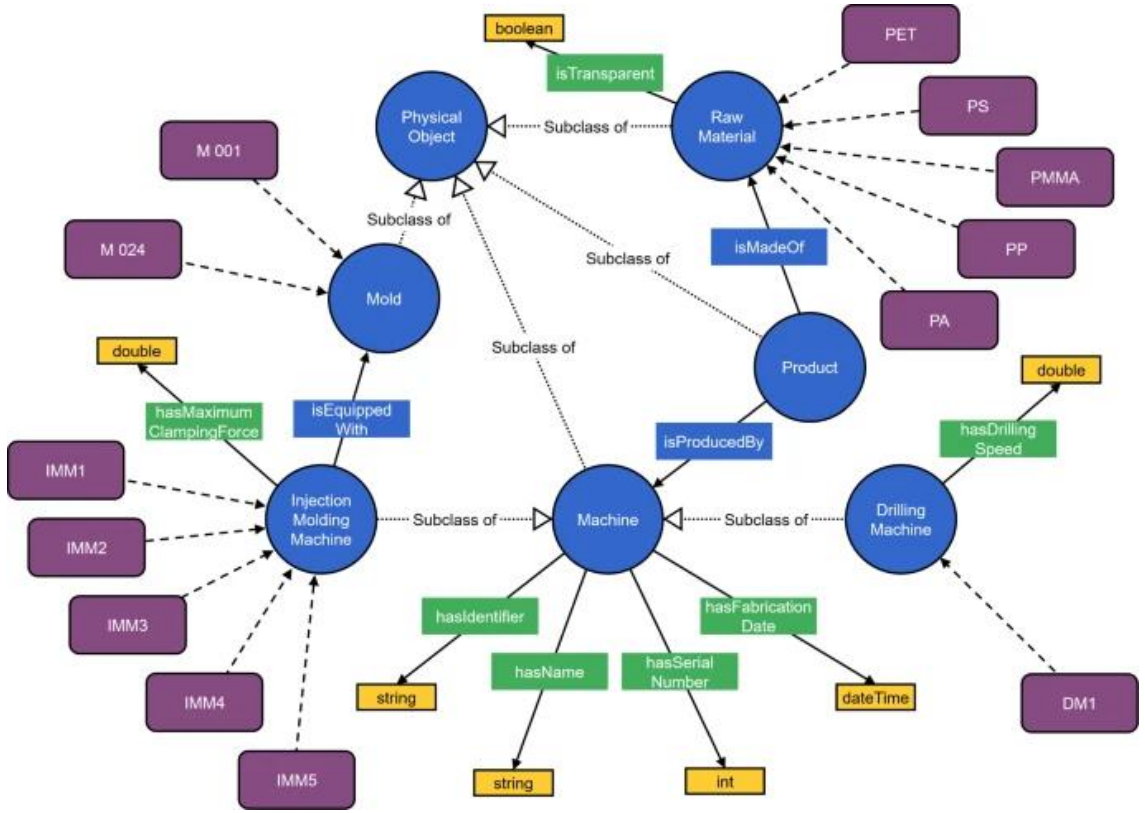
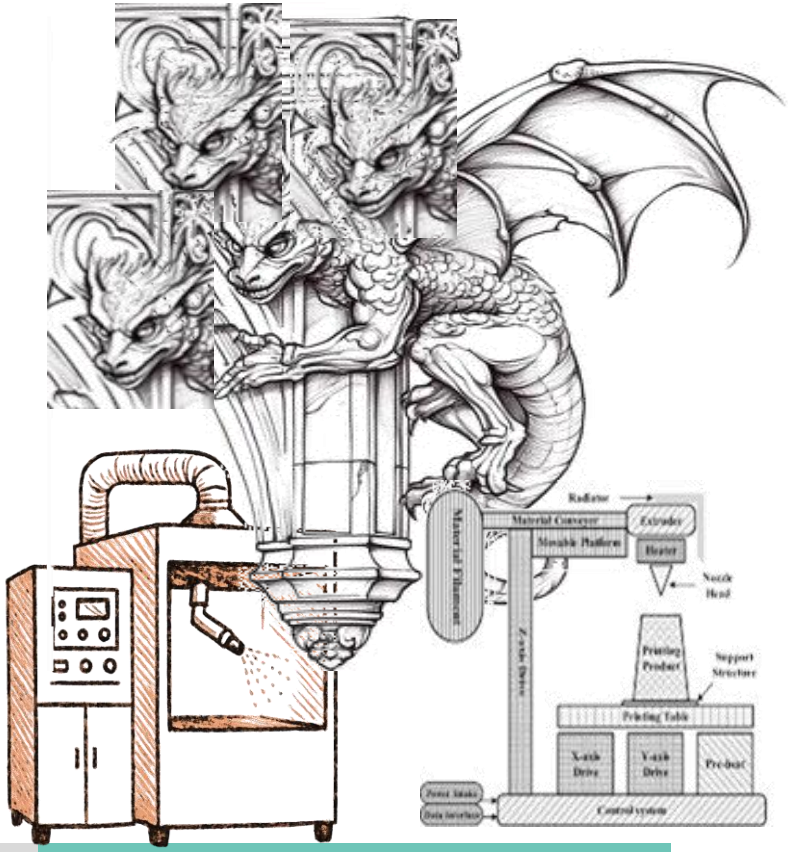
Controlled vocabularies (EMMO, AMLO, AMO, AWARE, CDOJP, COMP, CMCD)...>**65** manufacturing ontologies.



I potion

The Factory of Forgotten Fields

"Great machines roar, but no one writes down their secrets..."



Enemy: "The unknown process"

Difficulty: 10/10

-Occupational Exposure Ontology (**ExO** later →OExO, OccO, ENVO)

-ExO, is extended to human exposure to consumer product **LciO**

Sapel, P et al. (2024). https://doi.org/10.1007/s10845-024-02425-z,
https://zenodo.org/records/4665253#.YOlza-hKguU
https://www.mdpi.com/2079-4991/11/7/1818#B15-nanomaterials-11-01818

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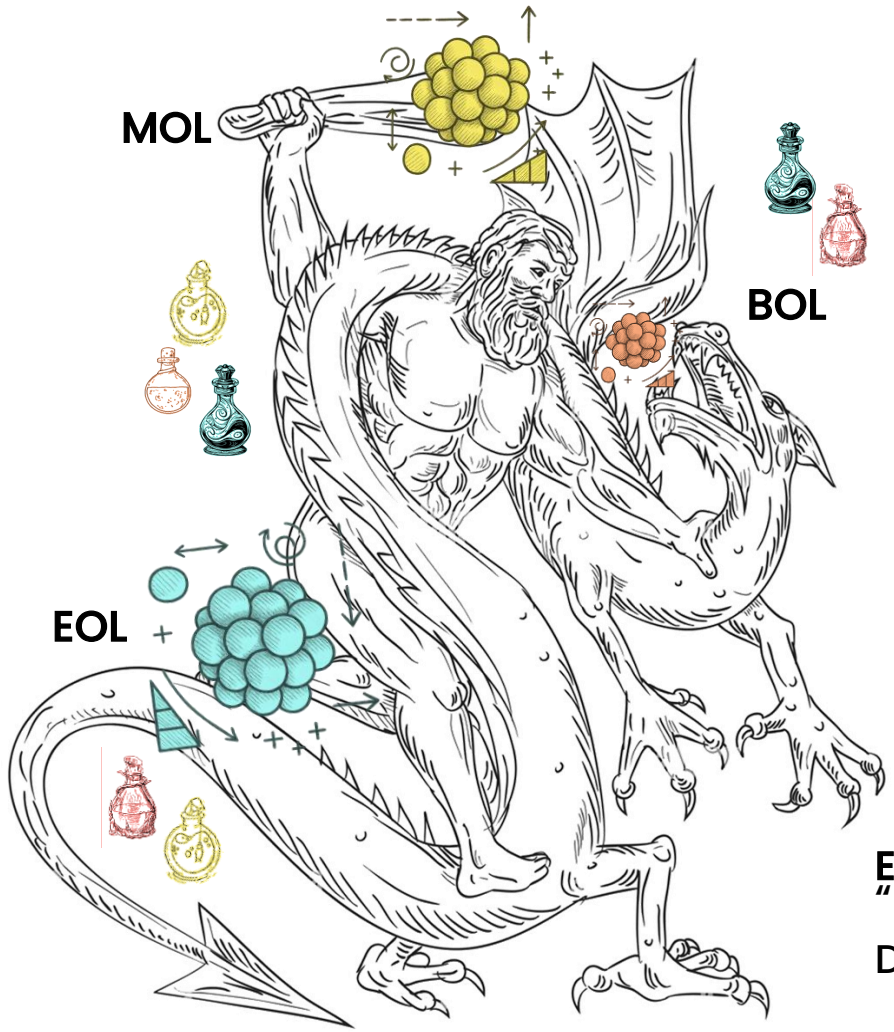
“Real World Meets Dragons”

3 main phases of the product life cycle.

- BOL includes planning, design, and manufacturing (LCS1-LCS2).
- MOL includes distribution (LCS2), use (LCS3), and support (e.g., repair and maintenance). Here the product is typically in the hands of the customer.
- EOL occurs where products are re-collected in the company’s hands in order to be recycled, disassembled, remanufactured, reused, or disposed (LCS4).



FAIR challenge: interdisciplinary data: material properties, product integration, human use, release, environment, recycling; circularity.

Enemy: “Prodactor”

Difficulty: 12/10

Funded by the European Union

“Real World Meets Dragons”

The Digital Product Passport (DPP)

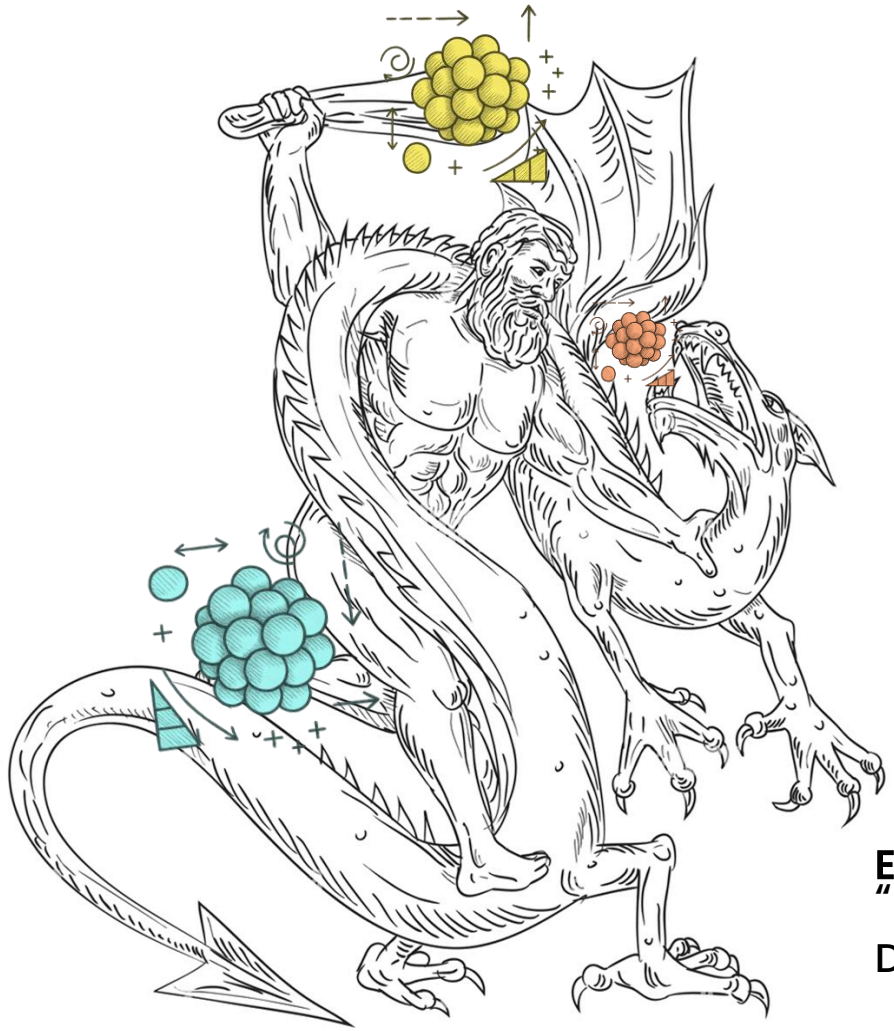
An initiative designed to improve transparency across product life cycles.

DPPs are anticipated to be adopted by the EU and mandated between 2026 and 2030

DigiPass

BOL MOL EOL

Digital Materials & Product Passport (DMPP)



Enemy: “Prodactor”

Difficulty: 12/10

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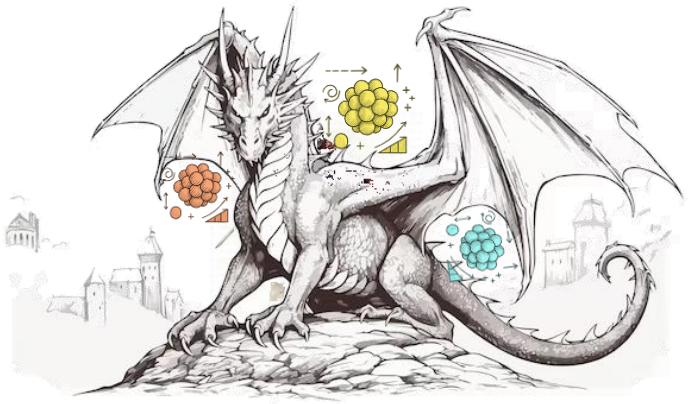
The Fellowship of FAIR

"One cannot fight dragons alone…"



The knowledge keepers

Data creators

Experimentalists, modelers, manufacturers

Data annotators

Ontology Engineer, Semantic Modeler

Data curators

Digital repository managers

Data integrators

Modelers, data scientists, policy teams, software developers

Data Shepherd/ Steward

All in 1 for 50% less price

"open educational resources" ELIXIR FAIR Cookbook and the NanoCommons UserGuidance Handbook

Funded by the European Union

What a tiny Victory looks like

1. Grant agreement by heart

NMs related aspects - SYNTHESIS | **Process related aspects - MANUFACTURING** | **END-OF-LIFE** | **Synthesis Manufacturing**

Process agnostic | **NEPs related aspects - USE**

Molecular re-design

Quality | Functionality | Sustainability | Intrinsic Hazard | Occupational Aspects | Consumers Aspects | End-of-life phase | Economic Sustainability

NMs related aspects | **NEPs related aspects - USE**

Design of Experiments | **AOP strategy** | **Human & Environmental related aspects** | **Optimization – Empirical & Digital Twins**

Process related aspects

Dimensions

Standards

UNI EN 1040:2006
ISO 14044:2006
OECD principles

MTT, OECD 487, WST1, LDH, ALAMAR, COMET, 53BP1, FET, ANNEXIN, H2AX

ISO 12947-2, ASTM E2149-13, Tiered exposure modelling

ISO 105 X12:2016 - Part X12, tiered exposure, OECD 439, ISO/TC 194/WG

LCC / LCA

EPA Standard Method 1311

Data

Quality Assurance
Functional NMs
Selectivity Index
Sustainability

pchem properties

ΣKPI: Intrinsic Human Hazard Composites

ΣKPIs: Intrinsic Environmental Hazard Composite

pchem properties

Functionality
Quality Assurance
Occupational safety
Population safety
Environm. safety

NEP

Human safety Release-intake-hazard

Environm. Safety Release-PEC-Fate-hazard

Leaching (landfilling)

Electrical energy and capital goods. Functional unit defined

Washing cycles & abrasions cycles – use based

Furxhi, I., et al. (**2024a**). Comput Struct Biotechnol J. https://doi.org/10.1016/j.csbj.2024.06.013
Furxhi, I., et al. (**2024b**). Comput Struct Biotechnol J. https://doi.org/10.1016/j.csbj.2024.10.001

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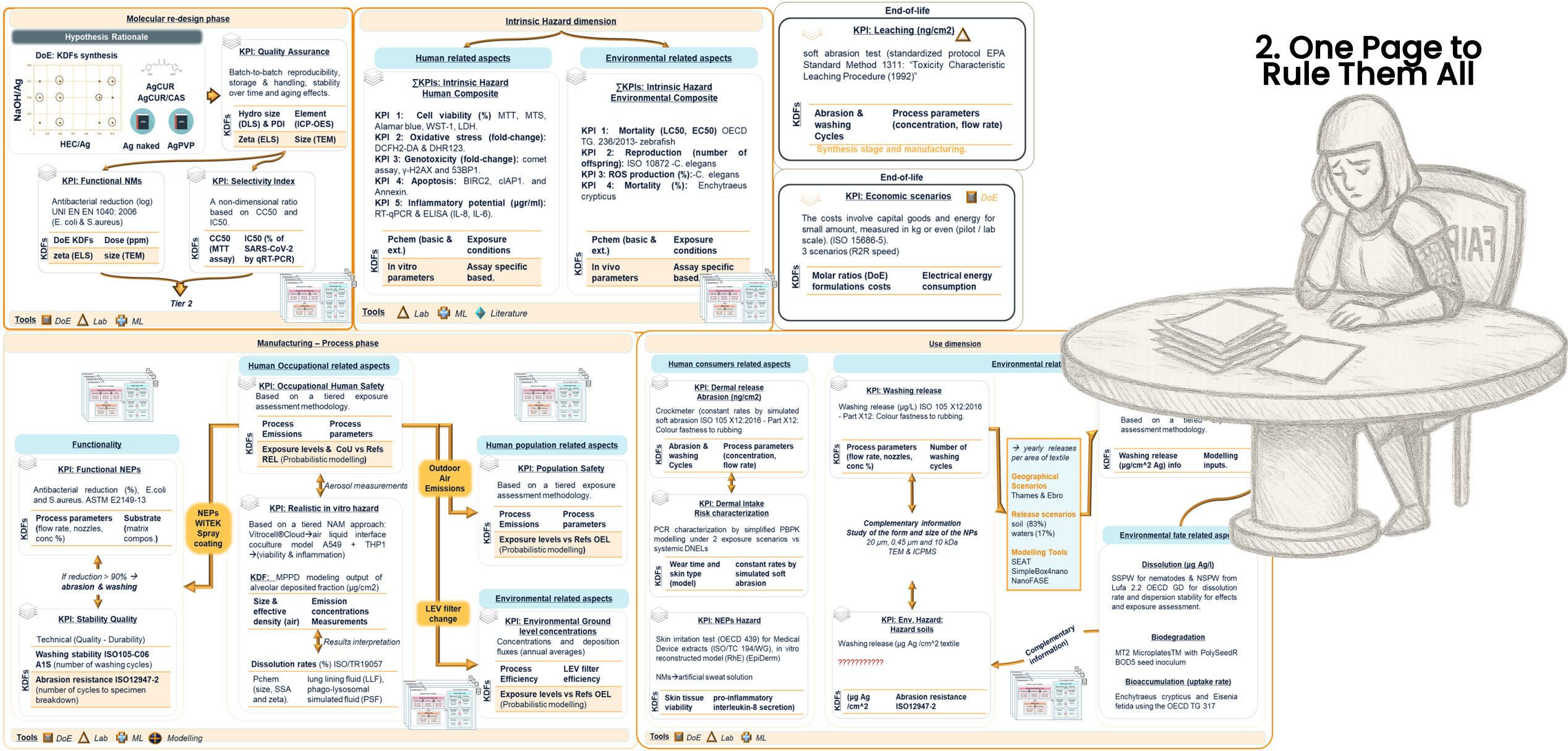
2. One Page to Rule Them All



Furxhi, I., et al. (**2022**). Frontiers in Bioengineering and Biotechnology 9. https://doi.org/10.3389/fbioe.2021.805096

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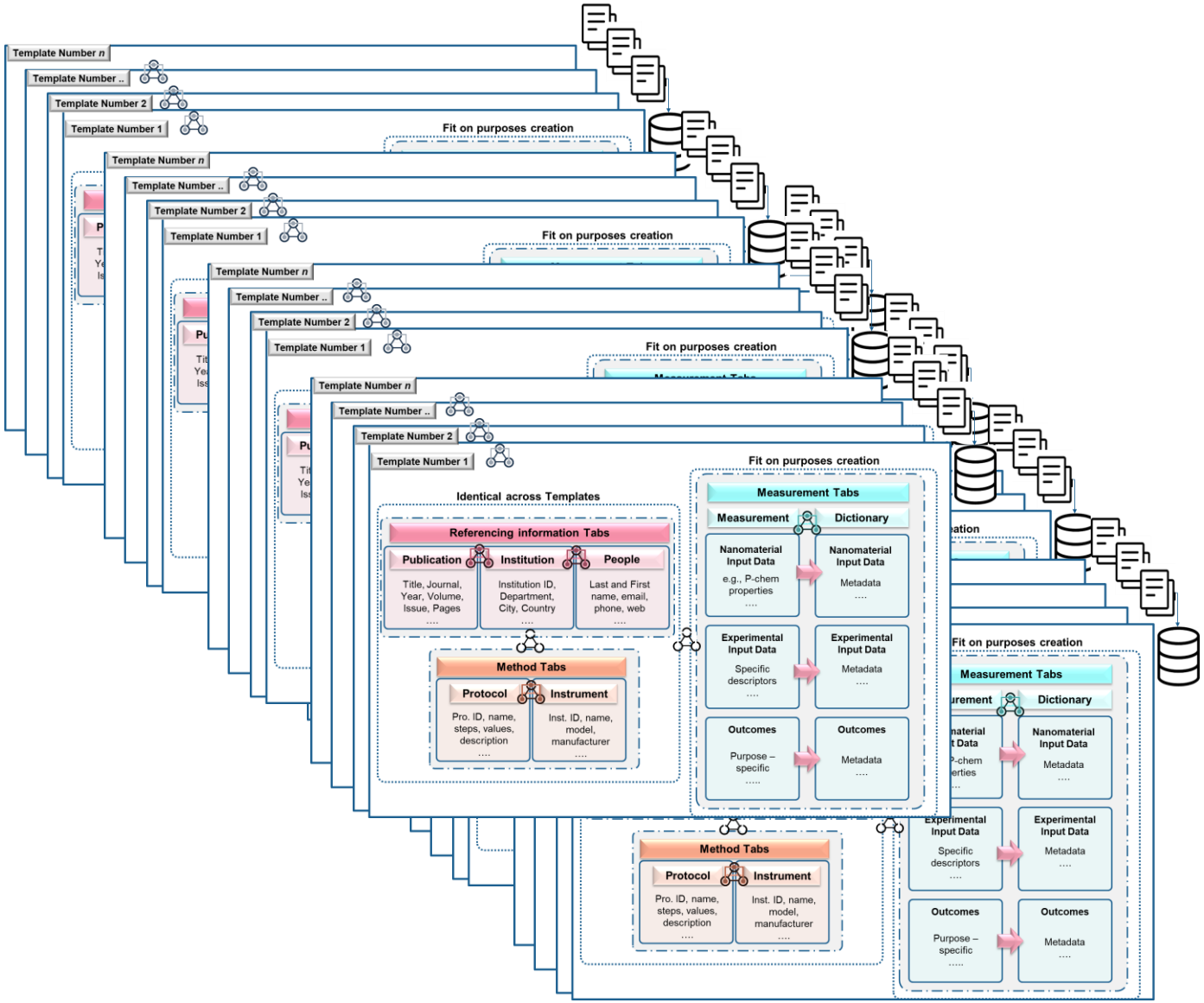
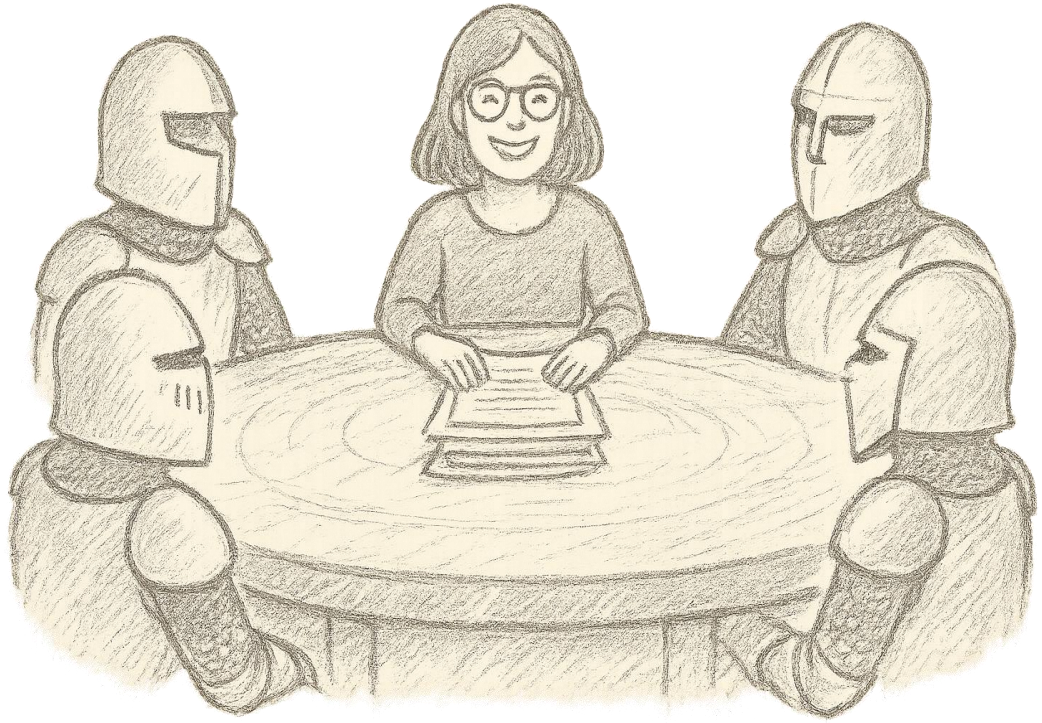


3. Involve all creators



Furxhi, I., et al. (2021a). Nanomaterials 11(6), 1520
Furxhi, I., et al. (2021b). Nanomaterials 11(7): 1818
Furxhi, I., et al. (2021c). Coatings 11(12): 1486

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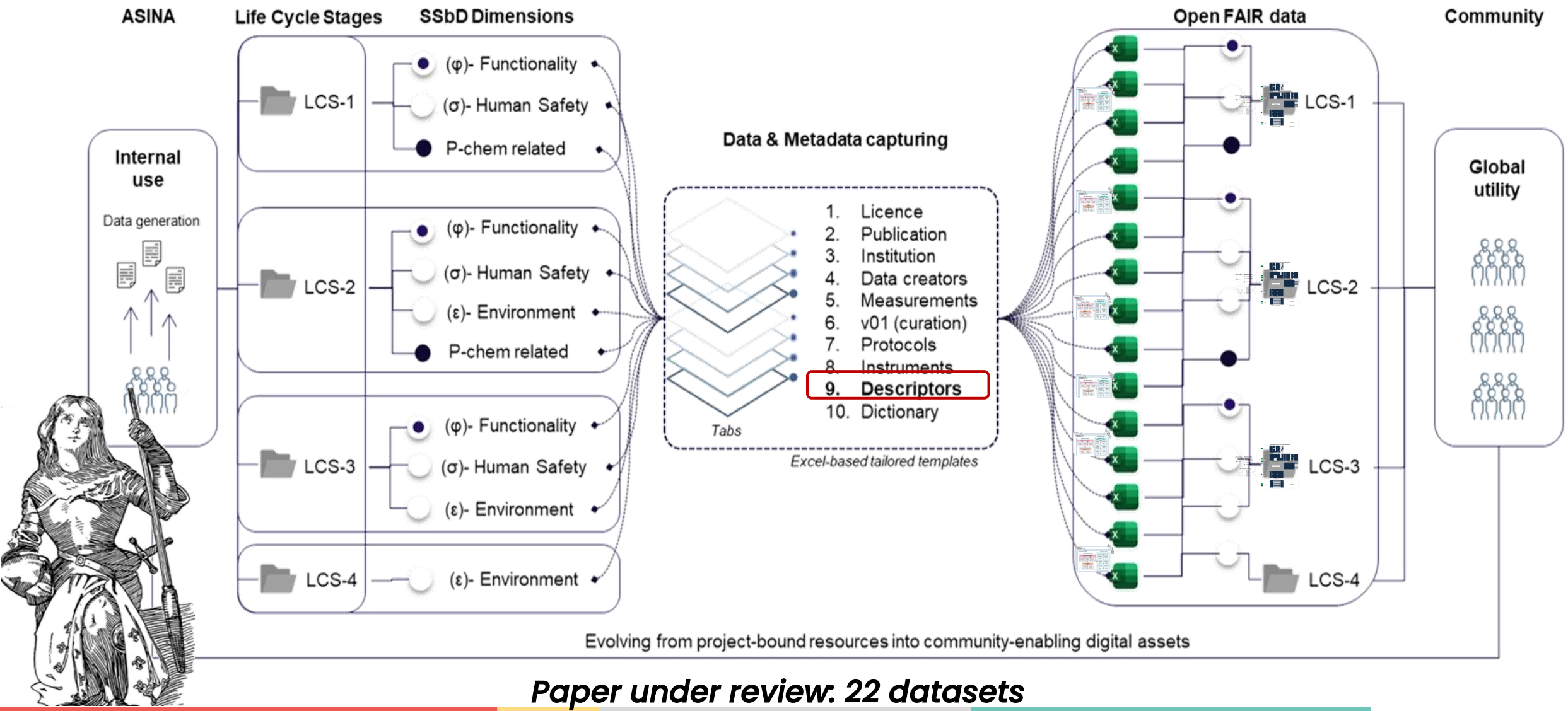
What a tiny medieval Victory looks like



Paper under review: 22 datasets

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What a tiny medieval Victory looks like

Nano Today 51 (2023) 101923

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/nanotoday

From principles to reality. FAIR implementation in the nanosafety community

Verónica I. Dumit [a,*], Ammar Ammar [b], Martine I. Bakker [c], Miguel A. Bañares [d], Cecilia Bossa [e], Anna Costa [f], Hilary Cowie [g], Damjana Drobne [h], Thomas E. Exner [i], Lucian Farcal [j], Steffi Friedrichs [k], Irini Furxhi [l,m], Roland Grafström [n,v], Andrea Haase [a], Martin Himly [o], Nina Jeliazkova [p], Iseult Lynch [q], Dieter Maier [r], Cornelle W. Noorlander [c], Hyun Kil Shin [s], Galo J.A.A. Soler-Illia [t], Blanca Suarez-Merino [u], Egon Willighagen [b], Penny Nymark [v,*]

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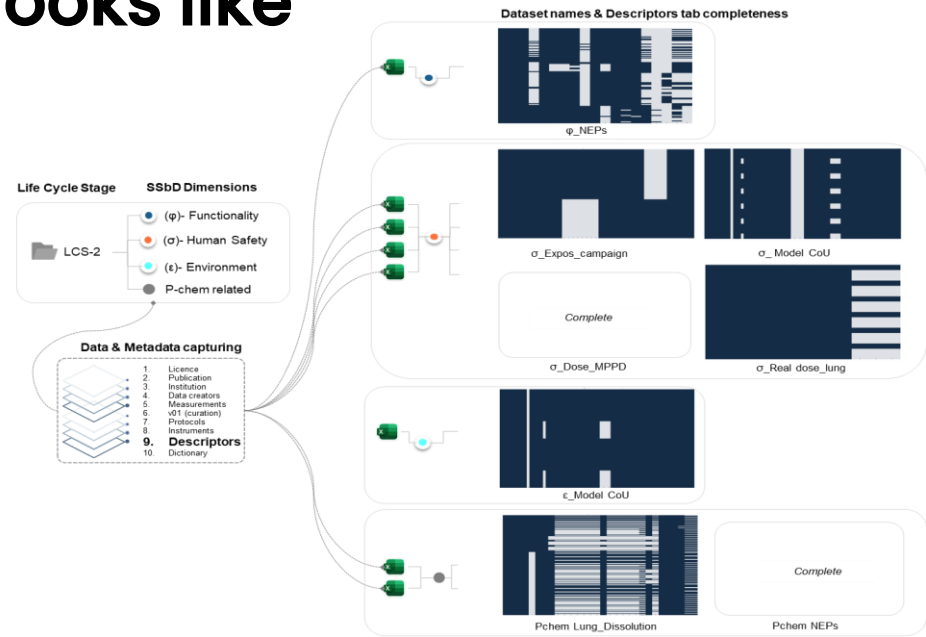
[d] Institute of Catalysis and Petrochemistry, Spanish National Council for Scientific Research (CSIC), Madrid, Spain
[e] Environment and Health Department, Istituto Superiore di Sanità, Rome, Italy
[f] ISTEC-CNR, Institute of Science and Technology for Ceramics, National Research Council, Faenza, Italy



nanomaterials MDPI

Nanomaterials (Basel). 2020 Sep 24;10(10):1908. doi: 10.3390/nano10101908

Your Spreadsheets Can Be FAIR: A Tool and FAIRification Workflow for the eNanoMapper Database

Nikolay Kochev [1,2,*], Nina Jeliazkova [2,*], Vesselina Paskaleva [1], Gergana Tancheva [1], Luchesar Iliev [2], Peter Ritchie [3], Vedrin Jeliazkov [2]

A forward-looking interpretation of the FAIR acronym;
"Findable and AI-Ready"
AdvancedNano IN

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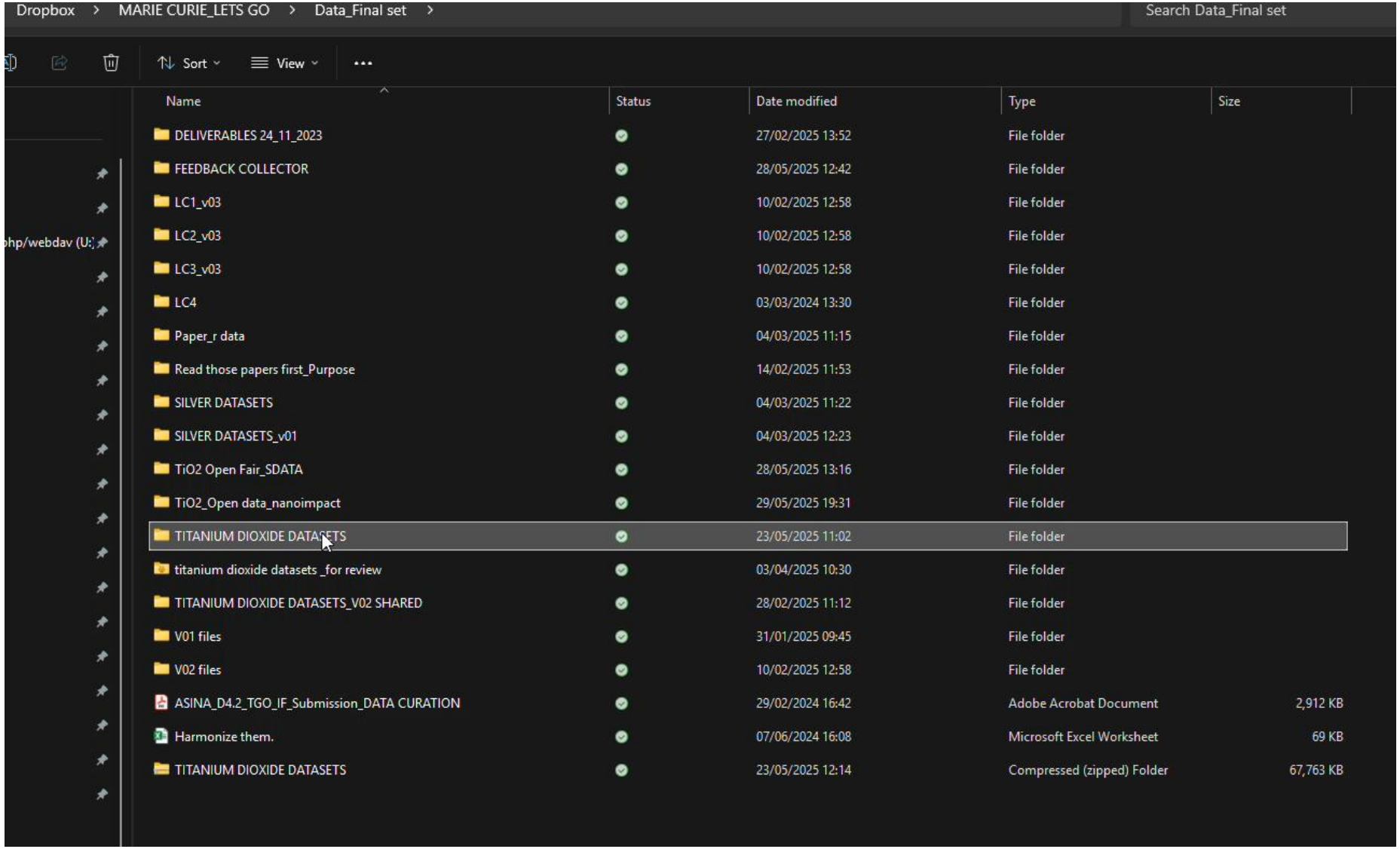

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Time flies, and so do the tools…

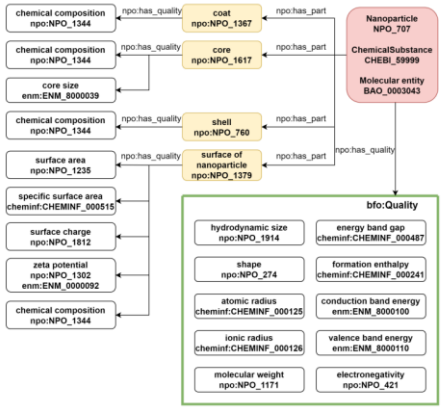
the Template Wizard

Template Designer Designing data entry templates for eNanoMapper

The Template Designer App is under development right now

Jeliazkova, N., *et al.* *Nat Protoc* **19**, 2642–2684 (2024). https://doi.org/10.1038/s41596-024-00993-1

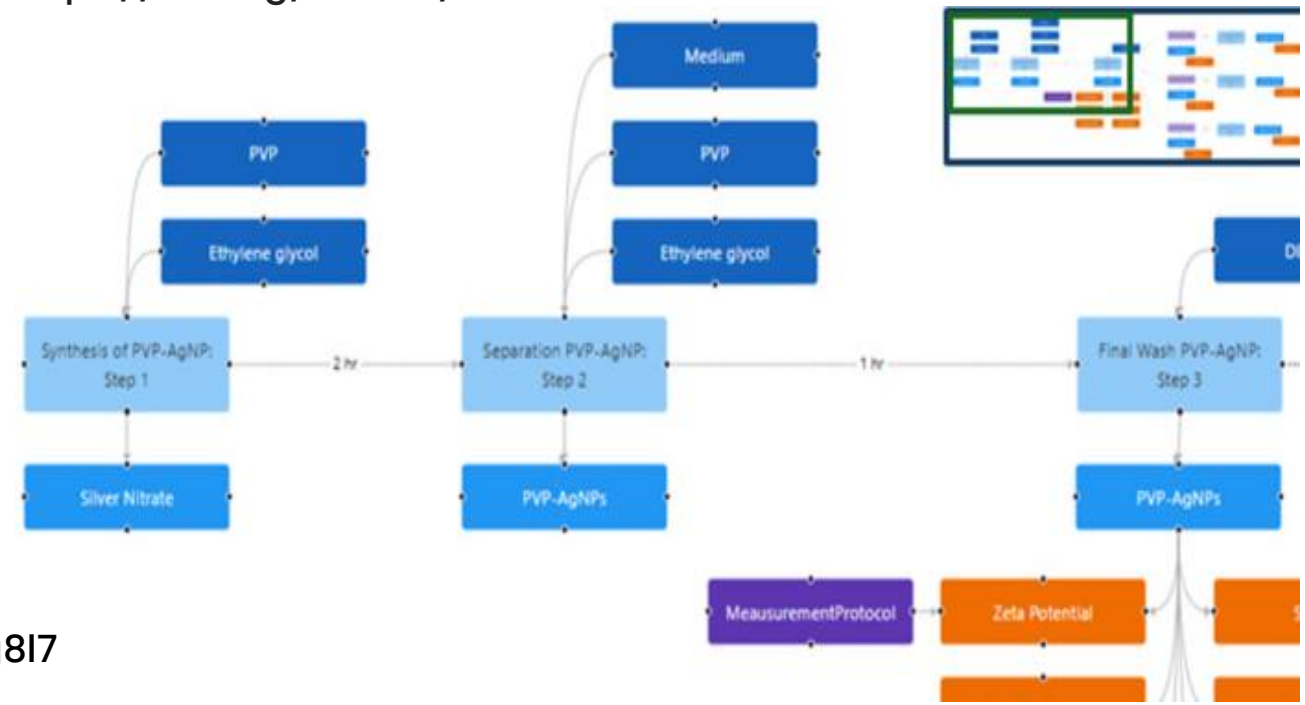
NanoSafety Data Reusability Assessment (NSDRA)



10.26434/chemrxiv-2024-lg8l7

Ammar, A., *Sci Data* **11**, 503 (2024). https://doi.org/10.1038/s41597-024-03324-x

NanoLinks



Punz B, . Beilstein J Nanotechnol. 2025 Jan 22;16:57-77. doi: 10.3762/bjnano.16.7. PMID: 39877837; PMCID: PMC11773194.

Instance maps and “on the fly”

Funded by the European Union

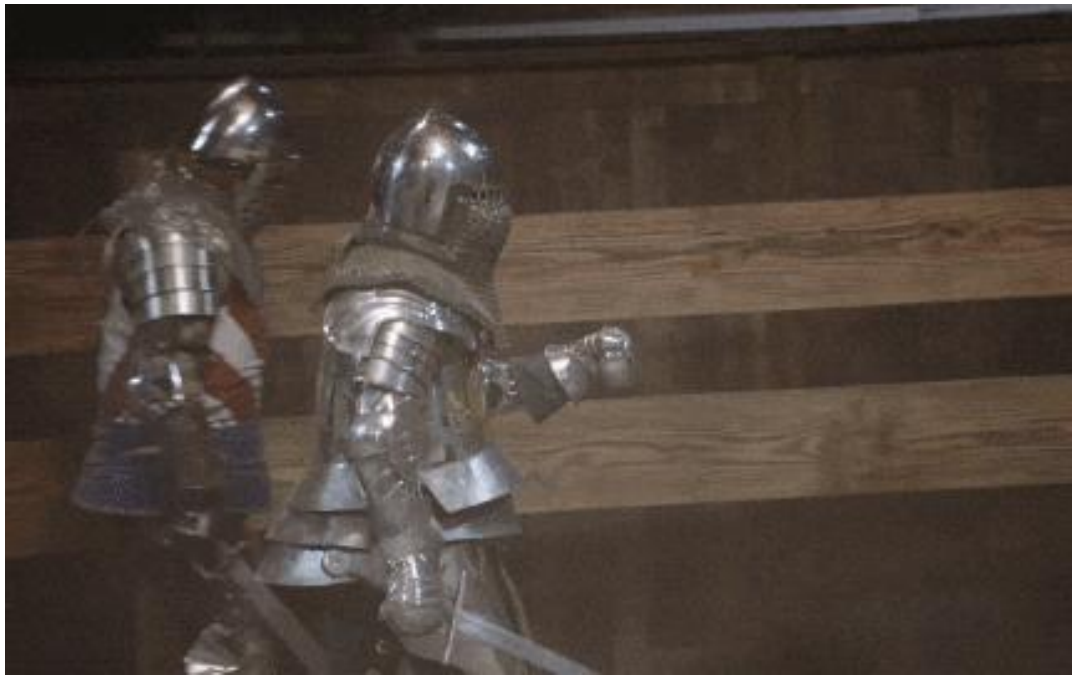
Final Reflections

Data hidden on hard drives help no one.

Even partially FAIR data can become a foundation for progress.

FAIRification is a continuous journey, not a binary state.

‘Ultimate FAIRness’? Aspirational—but worth striving for.



Managing data requires real effort: Before, During, After.

It’s not just about tools—it’s about collaboration, community, and commitment.

The data-sharing field remains far from perfected.

Funded by the European Union

I thank thee!

SAFETYFANS

SAFEty and sustainabiliTY by design Framework for Advanced Nano-Materials Synthesis

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