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Nano-Knowledge Community

The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

This project has received funding from the European Union Horizon 2020 Programme (H2020) under grant agreement no. 731032

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When is a metadata set complete?

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This project has received funding from the European Union Horizon 2020 Programme (H2020) under grant agreement no. 731032

Your most favoured piece of metadata

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Go to www.menti.com and use the code 89 55 42 8

Mentimeter

Relevant metadata

ninchi

1

Completeness

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3.1 Data completeness key concept (reproduced and adapted from [3]):

The completeness of data and associated metadata may be considered a measure of the availability of the necessary, non-redundant (meta)data for a given entity. However, there is no definitive consensus regarding exactly how data completeness should be defined in the nanoscience, or wider scientific, community. Indeed, metadata availability may be considered an issue distinct from data completeness.

3.2 Data quality key concept (reproduced and adapted from [3]):

Data quality may be considered a measure of the potential usefulness, clarity, correctness and trustworthiness of data and datasets. However, there is no definitive consensus regarding exactly how data quality should be defined in the nanoscience, or wider scientific, community. Data quality may be considered dependent upon the degree to which the meaning of the data is "clear" and the extent to which the data are "plausible". In turn, this may be considered to incorporate (aspects of) data completeness. For example, data quality may be considered to be (partly) dependent upon the "reproducibility" of data and the extent to which data are reproducible and their reproducibility can be assessed.

3. Robinson, R.L.M., Lynch, I., Peijnenburg, W., Rumble, J., Klaessig, F., Marquardt, C., Rauscher, H., Puzyn, T., Purian, R., Åberg, C. and Karcher, S., 2016. How should the completeness and quality of curated nanomaterial data be evaluated? Nanoscale, 8(19), pp.9919-9943.

FAIRness

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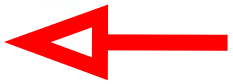
Box 2 | The FAIR Guiding Principles

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



FAIRness

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- To be **Reusable**:
  - SR1: Do not limit the reported metadata to fulfil only the requirements of the study for which the data was produced. Sections 6 and 7 provide examples on the re-usage of data in a different computational context than the experimental data producer initially intended.
  - SR2: Establish a feedback loop between data creators, analysts and customers to continuously improve the metadata completeness and quality. Keep in mind that scientific progress can lead to new use cases and go beyond "standards" defined at a specific point of time.

- To be **Interoperable**:
  - SI1: Provide direct links to descriptions of the test methods, protocols and quality control measures to give the user the chance to evaluate data interoperability. In this way, additional information, which cannot all be covered by the metadata can be easily accessed.
  - SI2: Report protocol metadata in a structured and annotated way to allow harmonisation and interlinking of data. While duplication of information in the protocol and the metadata is sometimes needed or even preferred, guarantee consistency between both.

Nanomaterial identifier - InChI for nano

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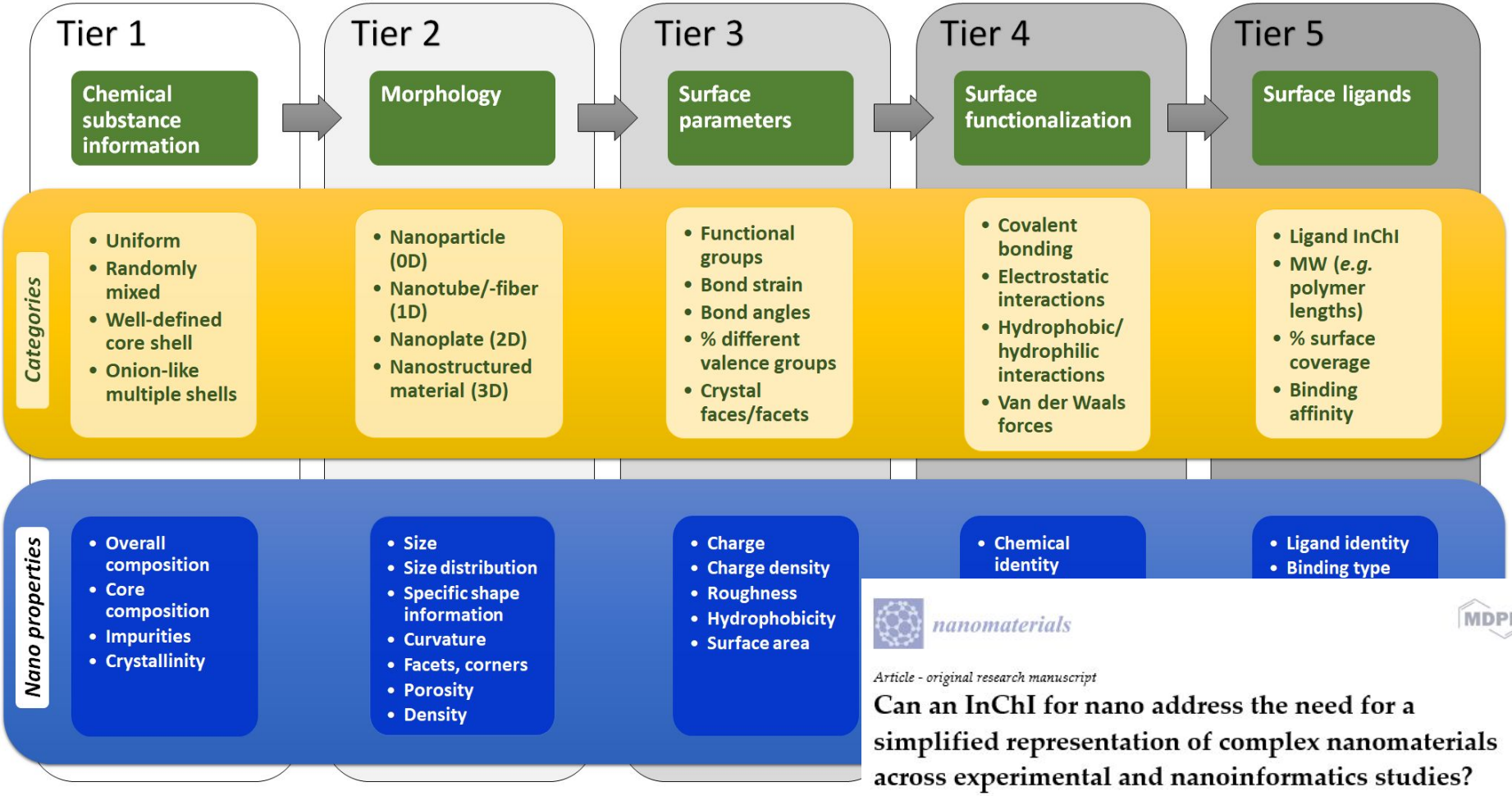


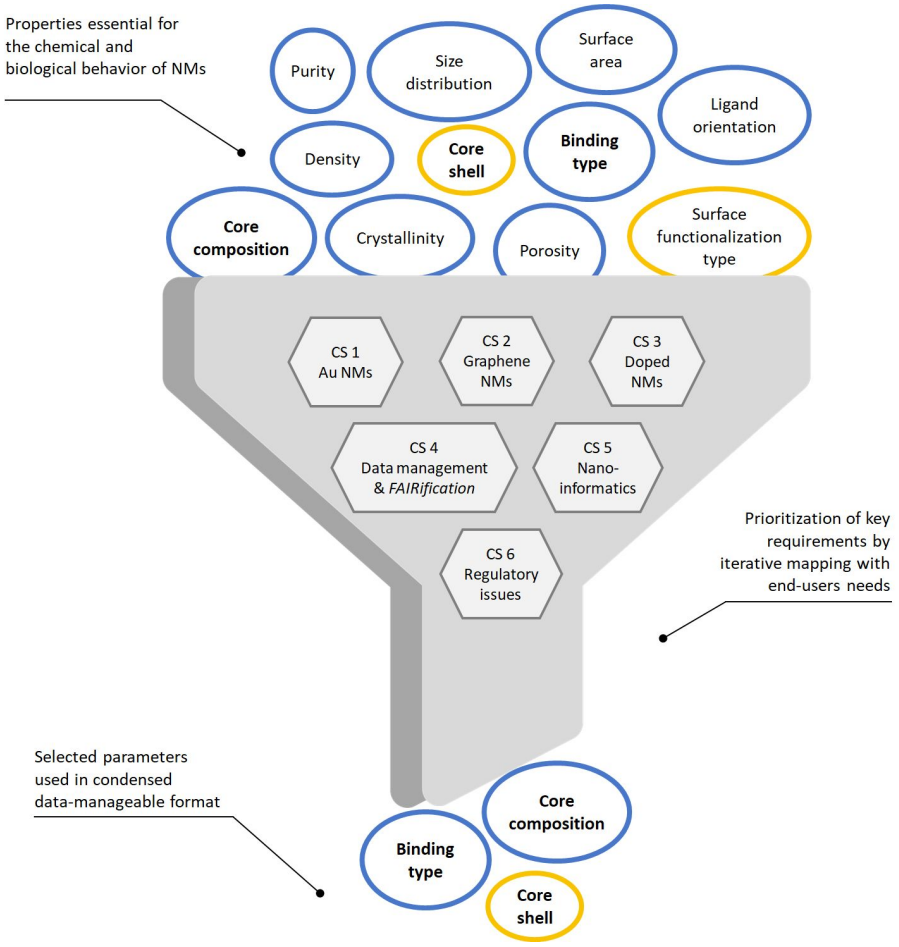
nanomaterials
MDPI
Article - original research manuscript

Can an InChI for nano address the need for a simplified representation of complex nanomaterials across experimental and nanoinformatics studies?

Iseult Lynch[1*], Antreas Afantitis[2], Thomas Exner[3], Martin Himly[4], Vladimir Lobaskin[5], Philip Doganis[6], Dieter Maier[7], Natasha Sanabria[8], Anastasios G. Papadiamantis[1], Anna Rybinska-Fryca[9], Maciej Gromelski[9], Egon Willighagen[10], Blair D. Johnston[11], Mary Gulumian[8], Marianne Matzke[12], Amaia Green Etxabe[12], Nathan Bossa[13], Angela Serra[14], Irene Liampa[6], Stacey Harper[15], Kaido Tämm[16], Alexander CØ Jensen[17], Pekka Kohonen[18], Luke Slater[1], Haralambos Sarimveis[6], Georgia Melagraki[2*]

Case studies

1. Library of Au NMs of different sizes and surface functionalities (ligands)
2. Library of carbon nanotubes
3. Complex chemistries and structures
4. NM-related data management and incorporation into the FAIR data landscape
5. NInChI in Nanoinformatics
6. Regulatory challenges



InChI for nanomaterials

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Category 1: must have	Category 2a: nice to have	Category 2b: extrinsic properties	Category 3: out of scope
• Chemical composition • Size / size distribution • Shape • Crystal structure • Chirality • Ligand and ligand binding	• Structural defects • Density • Surface composition	• Surface charge • Corona • Agglomeration state • Dispersion	• Optical properties • Magnetic properties • Chemical state / oxidation state

CTAB-capped-gold nanoparticles, diameter=20 nm:

NInChI=1A

/Au**/msp/s20d-9**

!C19H42N.BrH/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4;/h5-19H2,1-4H3;1H/q+1;/p-1

/y1&2

Data management, data lifecycle & metadata

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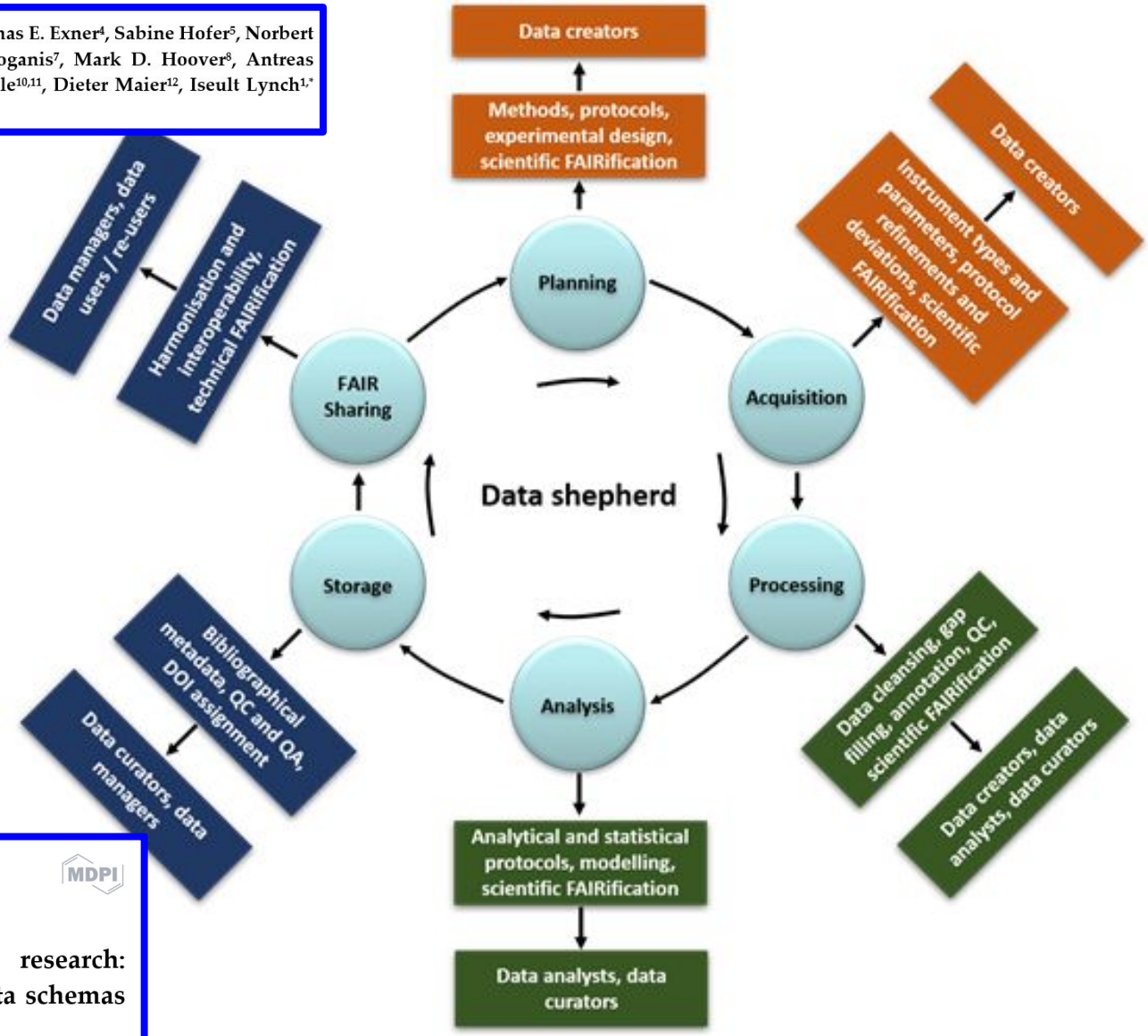
Anastasios G. Papadiamantis[1,2,*], Frederick C. Klaessig[3], Thomas E. Exner[4], Sabine Hofer[5], Norbert Hofstaetter[5], Martin Himly[5], Marc A. Williams[6], Philip Doganis[7], Mark D. Hoover[8], Antreas Afantitis[2], Georgia Melagraki[2], Tracy S. Nolan[9], John Rumble[10,11], Dieter Maier[12], Iseult Lynch[1,*] and members of the NCI nanoWG



nanomaterials
MDPI
Article

Metadata stewardship in nanosafety research: community-driven organisation of metadata schemas to support FAIR nanoscience data

Responsibilities

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Table 1. Data roles, responsibilities and interactions. Adapted from Hoover et al. [30,41] and Woodall et

	Set objectives	Design Approach	Collect	Processing	Modelling/Analysis	Validate	Store	Sh
Creators	X	X	X	X		X		
Analysts		X		X	X	X		
Curators				X		X		
Managers							X	X
Customers	X							
Shepherds	X	X	X	X	X	X	X	X

Metadata templates - the NanoFase case

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Instance Map

Terrestrial Mesocosm Experiment

protocolId	step ID	name	referencingId	durationValue/Unit	durationUnits	description	reference
1		Acid digestion				for fly ash samples	
	1	sample	1			dry powder	
	2	sample weight	1			20 mg	
						6 mL	
						1 mL	
						0.1 mL	

Protocol | Instrument | dictionary

Elemental Composition (wt. %)

datasetId	Ti	O	Na	Cl	Morphology	Specific Surface Area (m2/g)	Specific Surface Area StDev (m2/g)	Crystal Structure	TiO2 nanotubes concentration (µg/mL)	TiO2 con
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	InstrumentIB3		tase	0.00	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	BET		tase	6.25	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	126.9	0.6	Anatase	12.50	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	126.9	0.6	Anatase	25.00	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	126.9	0.6	Anatase	50.00	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	126.9	0.6	Anatase	100.00	
01.001/1000	41.1	58.9	< 0.05	< 0.05	Nanotubes and nanorods	126.9	0.6	Anatase	200.00	

Publication | Institution | People | Measurement | Protocol | Instrument | dictionary

NanoInformatics:

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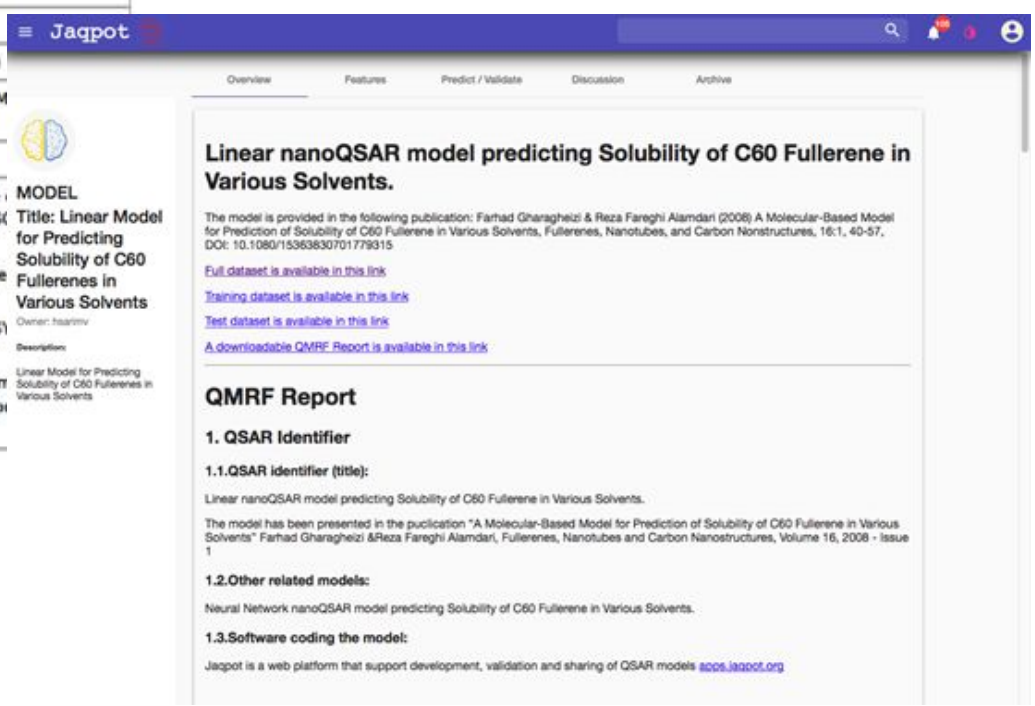
MODA

Elements in materials modelling

NANODOME

THE SIMULATION			
1	USER CASE	Nanoparticle synthesis via gas phase condensation in industrial commercially-relevant processes. Prediction of the nanoparticle size distribution, morphology and internal composition via modelling of the gas phase condensation synthesis process, including homogeneous and heterogeneous nucleation, surface and internal chemical kinetics and composition, agglomeration, aggregation. Materials: Si, ZnO, Al_2O_3, Pt nanoparticles in $Ar/H_2/N_2/O_2$ atmospheres for synthesis processes in plasma, hot wall and flame reactors.	
2	CHAIN OF MODELS	MODEL 1	Electronic Density Functional Theory (Electronic)
		MODEL 2	Classical MD (Atomistic)
		MODEL 3	Coarse Grained Molecular Dynamics (Mesoscopic)
		MODEL 4	Fluid mechanics, Heat-Flow, Chemistry Reaction M Electromagnetism (Continuum)
3	PUBLICATION	N.A.	
4	ACCESS CONDITIONS	Electronic and Atomistic models are based on widely available or open-source licenses packages, such as Quantum ESPRESS ReaxFF, GROMACS, GARFFIELD. The mesoscopic model will be developed within the NanoDome under open-source license. Continuum models are based on the commercial package ANS and on the open-source package OpenFOAM. Interfacing libraries and the material database for Si/Ar systen open-source. Material database for reactive materials will be p under commercial license.	



Agglomeration-related metadata and metadata questionnaires

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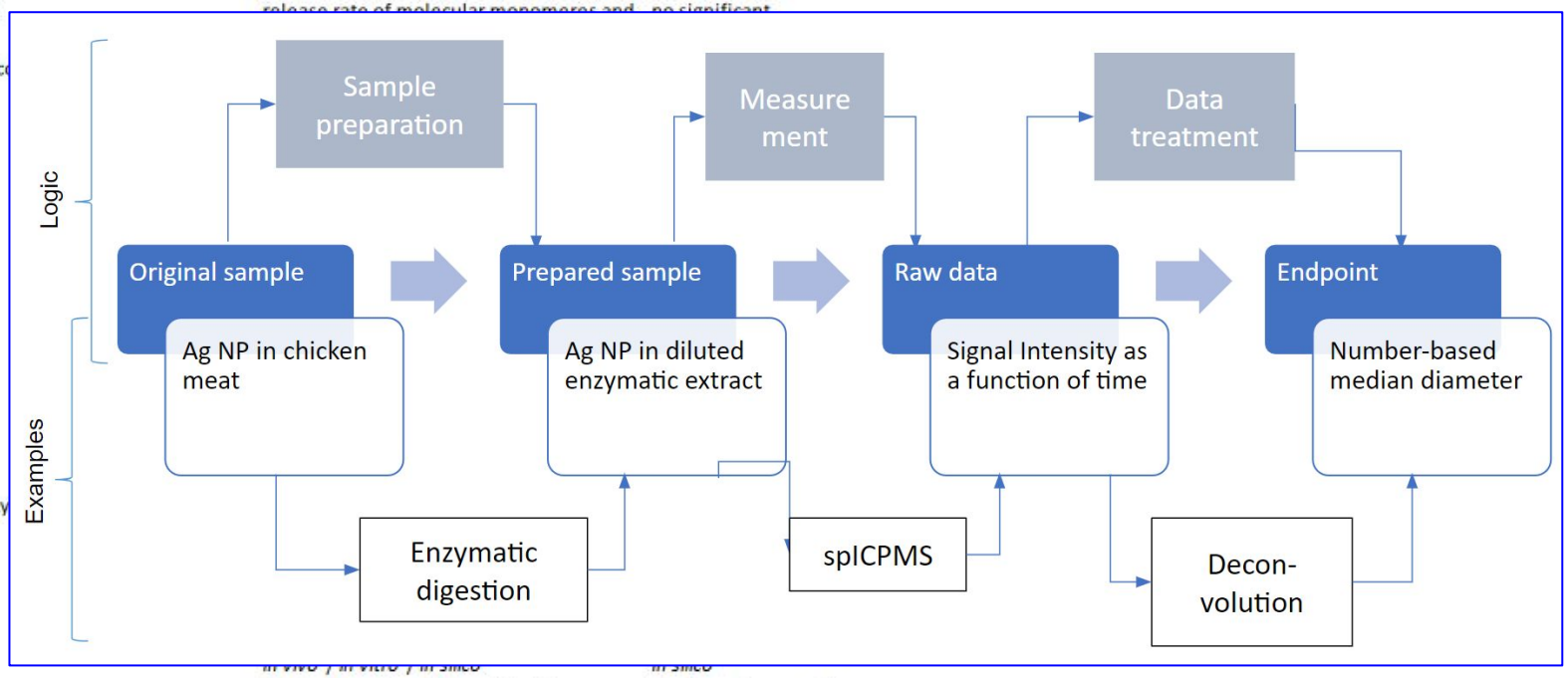
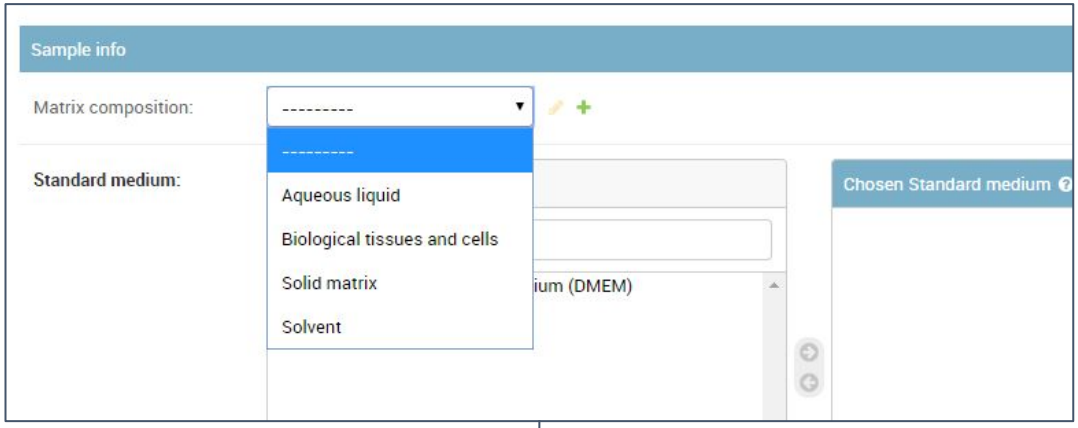
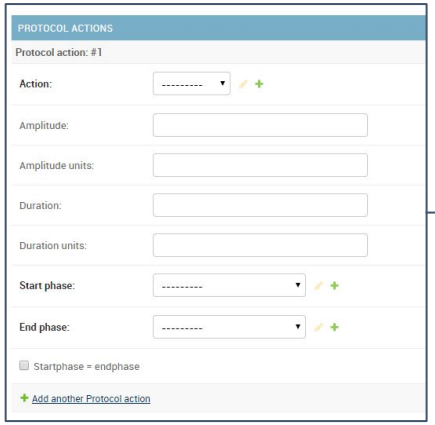
data object	NP descriptors	(meta)data	remarks / description	case study value	
primary particle	size	diameter	diameter of primary particle	50.0 +/- 0 nm	
		determination method	DLS, NTA, TEM, SEM, ...	NTA	
		statistical measure	mean, mode, median, ...	mean + stdv	
		size qualifier	hydrodynamic diameter, dried, ...	hydrodynamic diameter	
	shape		shape of particle (spherical, rod, ...)	spherical	
	aspect ratio		ratio of sizes in different dimensions	1	
	density		density of primary particle	SiO_2: 2.2 g/cm^3, TiO_2: 4.24 g/cm^3	
	surface charge		zeta potential of primary particle	-34 mV	*)
	porosity		pore volume fraction	non porous	
	polydispersity		polydispersity index, size distribution	monodisperse	
	dissolution rate		release rate of molecular monomeres and	no significant	
	synthesis protoc				
agglomerate	size				
	shape				
	aspect ratio				
	packing				
	effective density				
	polydispersity				
	stability				
experiment	method		in vivo / in vitro / in silico	in silico	
	model		for *in silico* only: which method is	*in vitro* , submerged,	



ACEnano web interface



- Capture details on chemistry of the original sample and the sample after preparation
- Definition and example of standard medium
- Some actions are complex and could be described separately (e.g. dispersion protocol including detailed steps and equipment used)



Original sample description

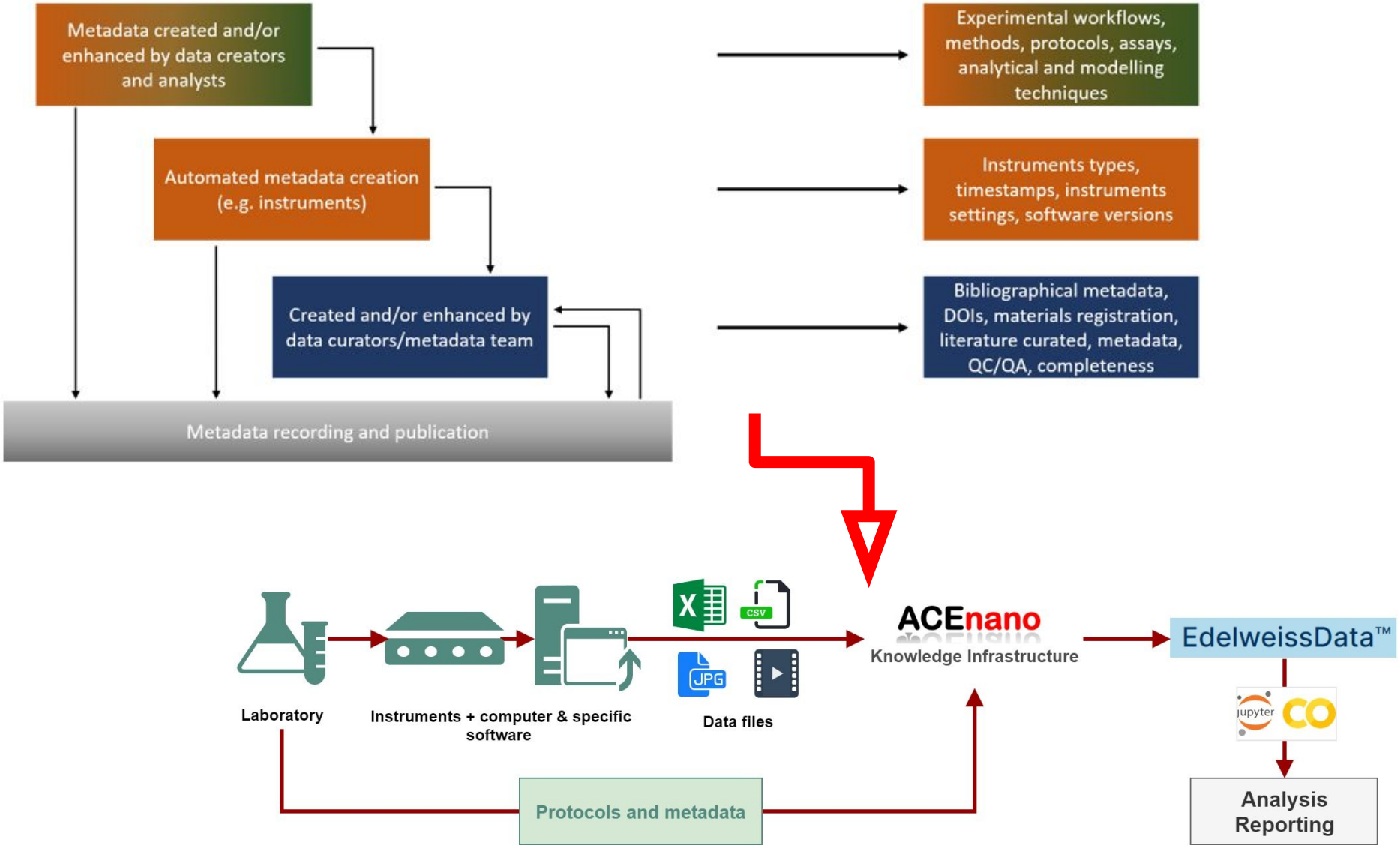
Dominant matrix composition of the sample: Solid matrix

Standardised media: Not applicable

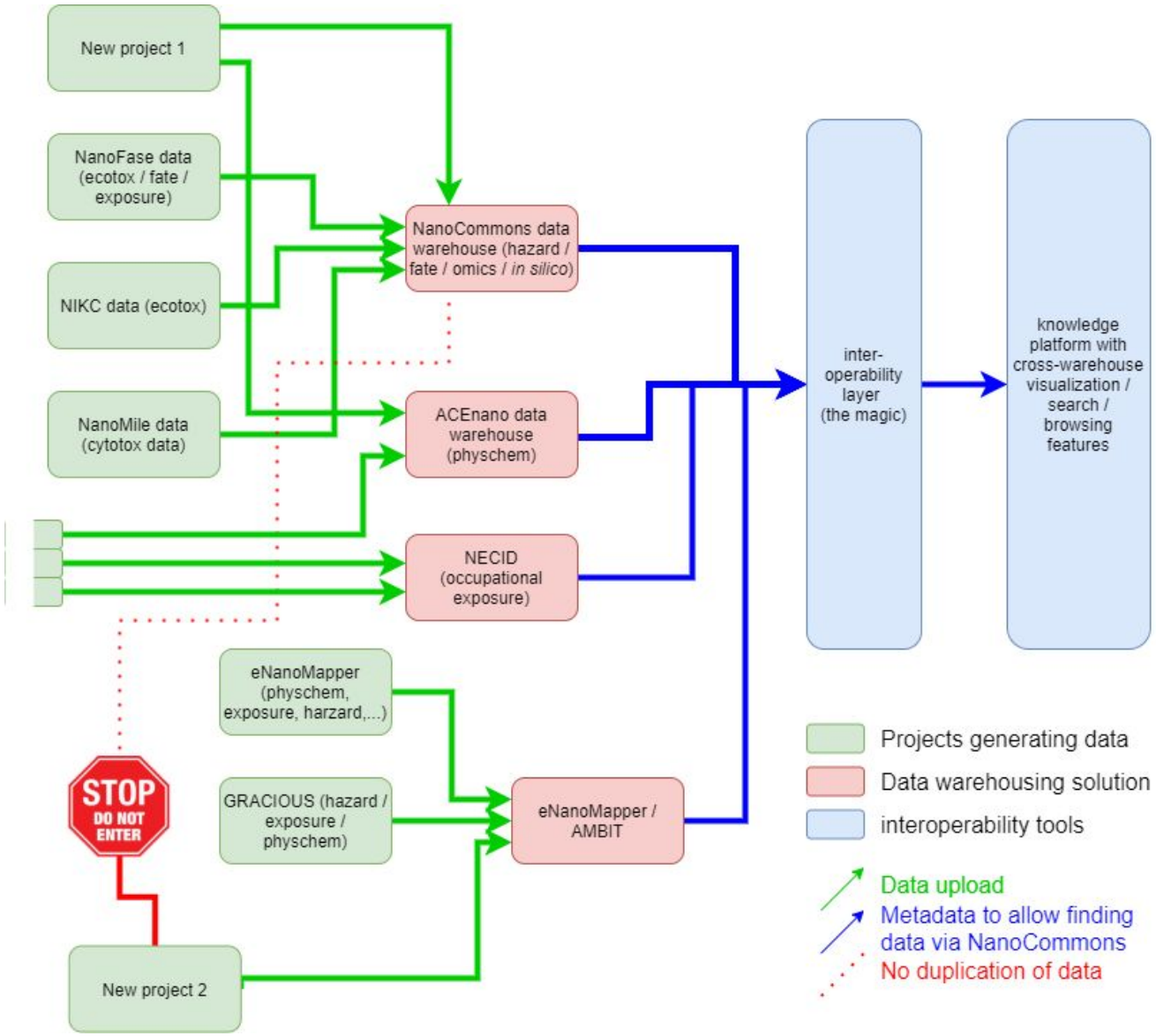
Sample preparation protocol

	Action name	Amplitude name	Amplitude	Amplitude units	Duration	Duration unit	Startphase
1	**Dispersion**	Compound	100	ml	None	None	Solid matrix
2	**Vortexing**	Vortexing speed	500	rpm	5	s	Aqueous liquid
3	**Sonication**	Frequency	1	Joule	5	min	Aqueous liquid

Upload workflows



And don't forget about semantics



The ontology development universe

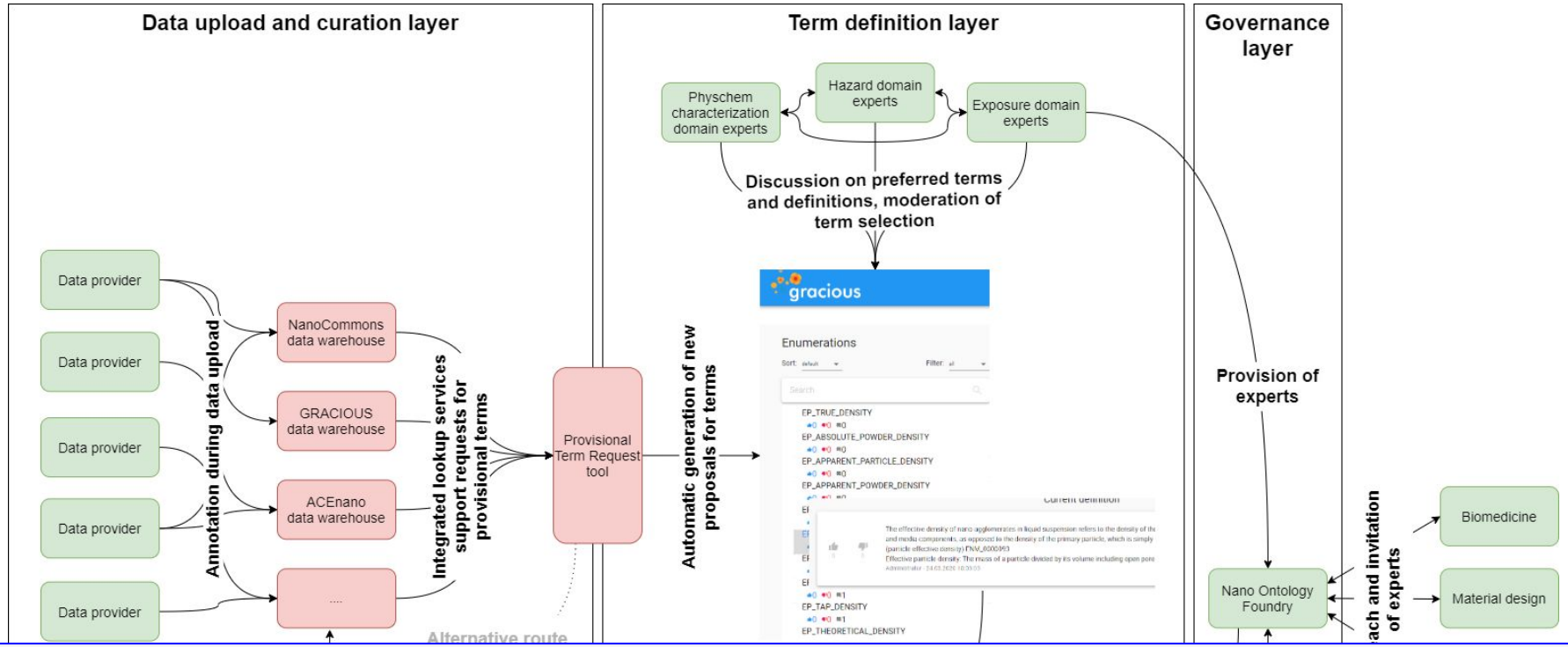


Table 2. Definition of the term "instance" for data creators, analysts, curators, managers, and customers.

Role	Example Term	Definition
Data creator	Experimental instance	A specific part of an assay or method
Data analyst	Training and test instances	A set of specific data entries used for training, testing and validating a predictive model
Data curator	NIKC instance	The reported nanomaterial in a system at a specific moment in time
Data manager	Database instance	A set of the background processes and memory structure needed by the database software to access the data
Data customer	All of the above depending on the specific use case	

When is a metadata set complete?

Never!?

But at least (minimal) standards should be defined and respected to cover most applications.

And these should improve over time.

Also based on new technology acceptable by all users.

Input from all sides are needed to achieve this!

Table 1. Data roles, responsibilities and interactions. Adapted from Hoover et al. [30,41] and Woodall et al. [42]. Adapted wi

	Set objectives	Design Approach	Collect	Processing	Modelling/Analysis	Validate	Store	Share	Quality Control	Anno	unication ducation
Creators	X	X	X	X		X			X		X
Analysts		X		X	X	X			X		X
Curators				X		X			X		X
Managers							X	X	X		X
Customers	X								X		X
Shepherds	X	X	X	X	X	X	X	X	X		X

Whatever your role is,

in the NSC WG F!

https://www.nanocommons.eu/ta-access/
https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi

Your most favoured piece of metadata

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Go to www.menti.com and use the code 89 55 42 8

Mentimeter

Relevant metadata

ninchi

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Thank you *for your attention!*

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Iseult Lynch
Tassos Papadiamantis
Dieter Maier
Egon Willighagen
Martin Himly
Danail Hristozov
Alex Zabeo
and many more

Joh Dokler
Lucian Farcal
Maja Brajnik
Barry Hardy

NSC Education Day @ NANOSAFE 2020,
16 November 2020

Whatever your role is,

in the NSC WG F!