A common European approach to the regulatory testing of nanomaterials

Data(management)

The approach in NANoREG and ProSafe

NIH nanoWG – 7 April 2016

Sara Totaro
Hugues Crutzen

EC - Joint Research Centre - Ispra site (Italy)
Partner in NANoREG and Prosafe

Outline

- ➢ Background for data logging

- ➢ 'Data activitites' in NANoREG and Prosafe
    - ➢ NANoREG T1.5 – key elements
    - ➢ Prosafe WP3 – key elements

- ➢ The concept of ISA-TAB-Nano / Json…

- ➢ In details
    - ➢ NANoREG T1.5 data platform
        - ▪ NANoREG data logging system
        - ▪ The templates
        - ▪ Way forward
    - ➢ Prosafe WP3
        - ▪ Prosafe support to the data-handling

The projects in short

NANOREG

- ➢ Large collaborative research in nanoEHS
- ➢ 4 years, >65 partner organisations
- ➢ EU-funded 20%, National funding 80%

ProSafe

- ➢ Coordination and support action (CSA) in nanoEHS
- ➢ 2 years, 11 partner organisations
- ➢ EU-funded at about 85%

Background

➢ Meaningful and comparable data to foster the assessment of quality and reliability of testing methods in nanoEHS

➢ To facilitate the data recording ('logging')

➢ To support linking and comparability of EU projects output

➢ To possibly integrate the 'templates system' with the one(s) built for SAR models in the context of safe-by-design (SbD)

'Data activities' in NANoREG and Prosafe

➢ **NANoREG T1.5** – Data platform and data(management) for the project

➢ **PROSAFE WP3** – Coordinate, support the streamlining of data acquisition, collection and linking

Under the leadership of JRC

T3.1 – Mapping databases

T3.2 – NanoEHS community-agreed database management system

sub-tasks

Sub-task 3.2.1
ISA-TAB-Nano as backbone
for a common database

Sub-task 3.2.2
Minimum requirements in ontology
and naming conventions

T3.3 – Linking databases

NANoREG T1.5 – Key elements

T1.5 – DoW – Data platform and data management

This task will develop the NANoREG data platform, by connecting or integrating to IUCLID-based databases (JRC-NanoHub). This includes: a) Setting-up the NANoREG data platform, b) Integration of existing data, documentation of reviewed sources, c) explore the possibilities to provide guidance on how to convert data based on different metrics, d) Integration of new NANoREG data. It will be investigated which query tools might be relevant/appropriate for such a database. Optionally, it is foreseen to integrate data from other DBs using the Federated data search approach and the integration of data from reviewed papers (e.g. NHECD). This task includes performing the coordination of how data and reports will be stored in the NANoREG data platform and providing presentation and answering possible questions to/from users of platform. These activities will be integrated and carried out in collaboration with the NANoREG web site to be developed in WP 7.

NANoREG T1.5 – Key elements

➢ Setting up the NANoREG internal data platform

- Integration of NANoREG data ➡ **NANoREG data logging system**

➢ Performing the coordination of how data and reports will be stored in the NANoREG data platform

NANoREG choice:
ISA-TAB-Nano logic as backbone

Prosafe WP3 – key elements

➤ Need to streamline data acquisition, collection and management within the 'nano-scientific' community

Sound and resource-efficient approach to data management

ISA-TAB-Nano as backbone for a common database
(T 3.2.1)

Minimum agreed ontology
(T 3.2.2)

DB-linking
(T3.3)

Exploitation of already existing DBs

➤ Support the promotion of the importance of *nanoinformatics*
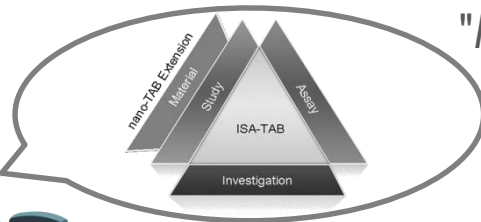
… and the JRC's role
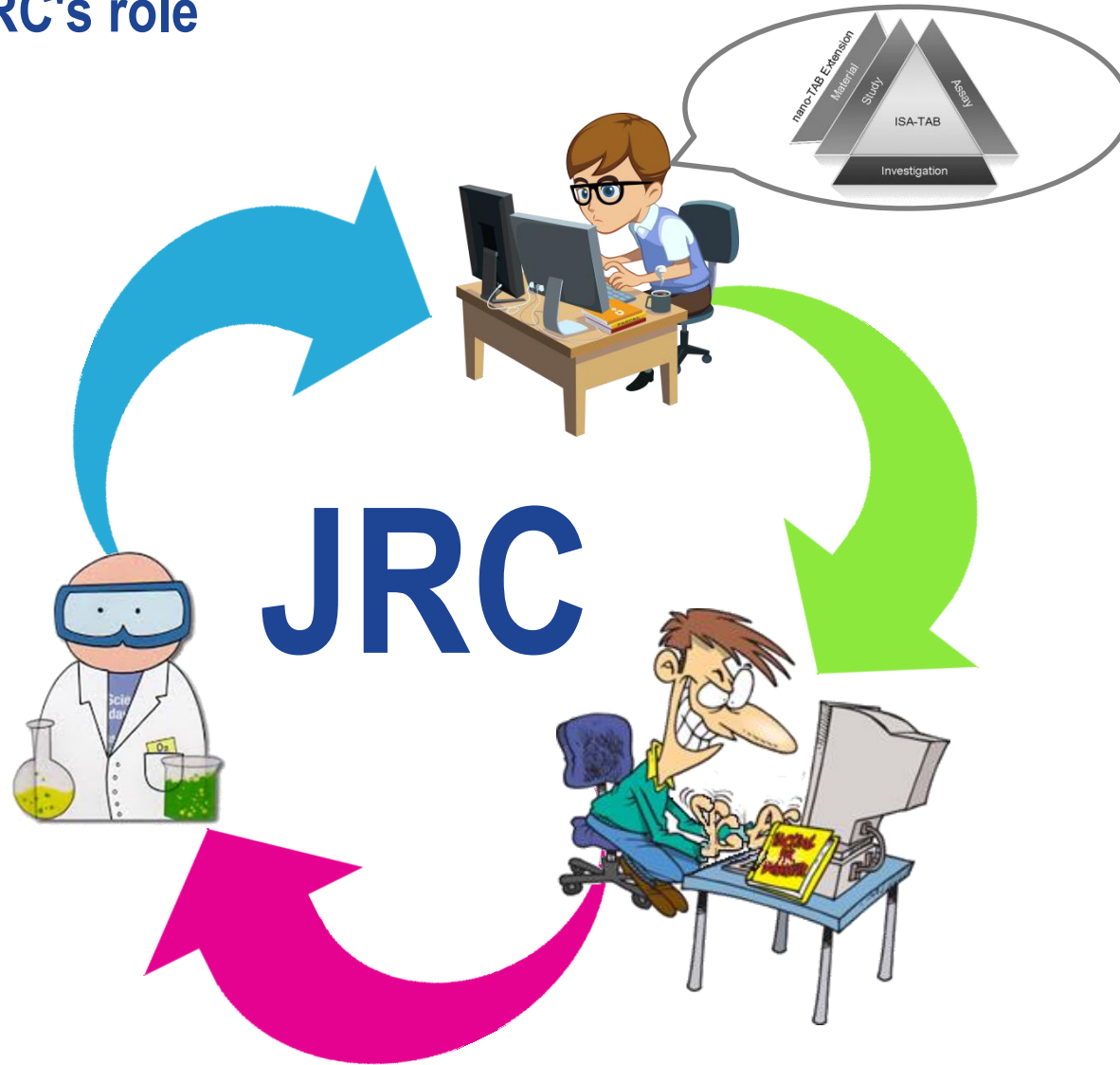
View details

NANoREG T1.5
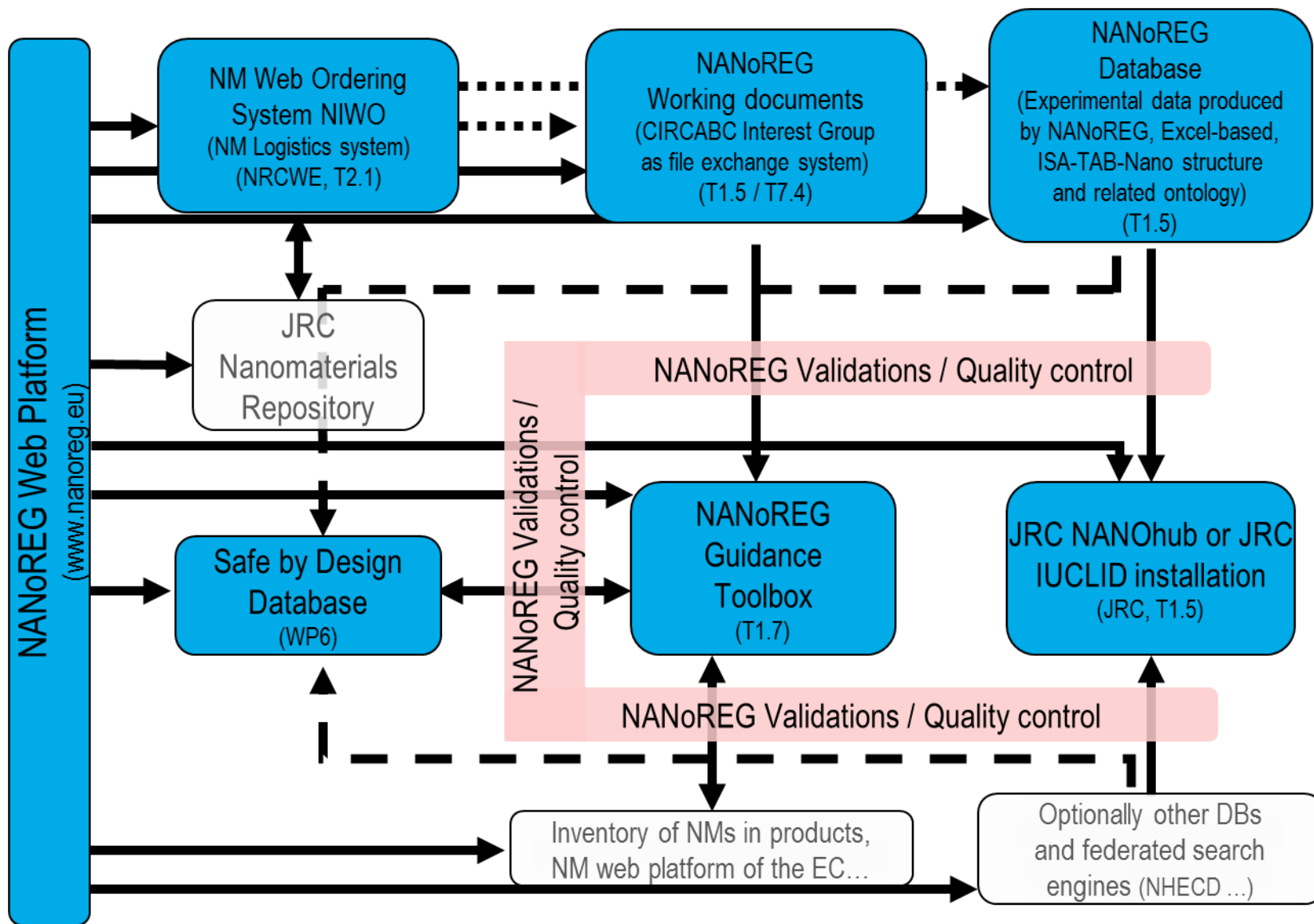
NANoREG data platform (structure as from Oct 2014)

NANoREG Web Platform (www.nanoreg.eu)

NM Web Ordering System NIWO (NM Logistics system) (NRCWE, T2.1)

NANoREG Working documents (CIRCABC Interest Group as file exchange system) (T1.5 / T7.4)

NANoREG Database (Experimental data produced by NANoREG, Excel-based, ISA-TAB-Nano structure and related ontology) (T1.5)

JRC Nanomaterials Repository

NANoREG Validations / Quality control

Safe by Design Database (WP6)

NANoREG Validations / Quality control

NANoREG Guidance Toolbox (T1.7)

JRC NANOhub or JRC IUCLID installation (JRC, T1.5)

NANoREG Validations / Quality control

Inventory of NMs in products, NM web platform of the EC...

Optionally other DBs and federated search engines (NHECD ...)

Greyed components are externally linked to the NANoREG platform and optional

NANoREG data platform (structure as from Oct 2014)

The JRC Nanomaterials Repository

More than 20 Representative NMs to support the scientific community/research in nanoEHS

Visit us at:

https://ec.europa.eu/jrc/en/scientific-tool/jrc-nanomaterials-repository

Greyed components are externally linked to the NANoREG platform and optional

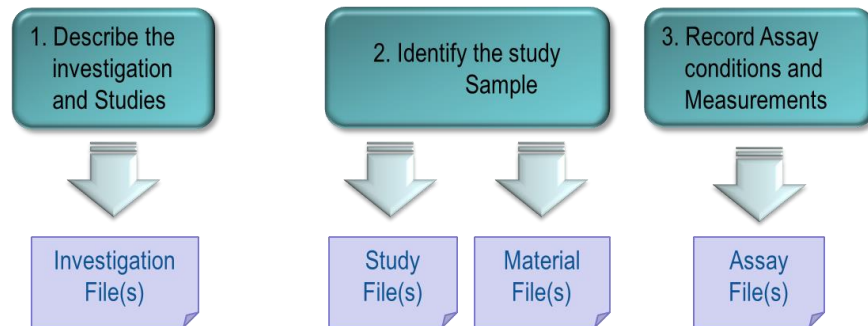# NANoREG data platform

Greyed components are externally linked to the NANoREG platform and optional

NANoREG data logging system - background

- ISA-TAB-Nano logic as backbone ➡ What it is and how it works

1. Describe the investigation and Studies	2. Identify the study Sample	3. Record Assay conditions and Measurements

Investigation File(s) | Study File(s) | Material File(s) | Assay File(s)

4 excel files containing a diverse number of 'entries/rows'

Investigation file: 105 entries
Material file: 16 entries
Study file: 28 entries
Assay file: 21 entries

In total 170 entries
Structured in different files

What goes where????

- The NANoREG data logging 'users' ➡ Mainly scientists

NANoREG data logging system - Implementation

- The NANoREG data logging 'users' ➡️ Mainly scientists

Build Excel®-based templates to log the experimental data produced in NANoREG WPs 2, 3, 4, 5 (Scientific WPs)

Phys-chem, *in vitro* and *in vivo* tox

Identification of meaningful parameters to describe an assay
Dialogue with our NANoREG experts and partners

The templates…

Sample Information		

Replicate number	NM ID code	Vial number	…

Ontology attributes

to be completed

Size distribution						

Dispersion protocol	Size Distribution (monomodal…)	Size distribution analyse method (ex: DLS, CLS, etc…)	Dispersion medium	Concentration (mg mL^{-1})	Mean Hydrodynamic diameter (nm)	in weight (w) or numer (n)*	PDI

Module (phys-chem, in vivo, in vitro)	Endpoint (e.g. OECD list, NANoREG relevant)	Assay / technique name (ex: DLS, MTS)	Protocol REF = SOP (ex: NanoValid MTS protocol)	Date of acquisition

The templates…

Experimental parameters						
Hydrodynamic Diameter (nm)	Cell model	Resting time at room temperature	Temp (°C)	Thermal equilibrium time (min)	Instrument Model	Number of runs
Number of sub-runs	Delay between runs	Laser focus position	Laser attenuation	Scattering angle	Refractive index of the sample	Absorption index of the sample

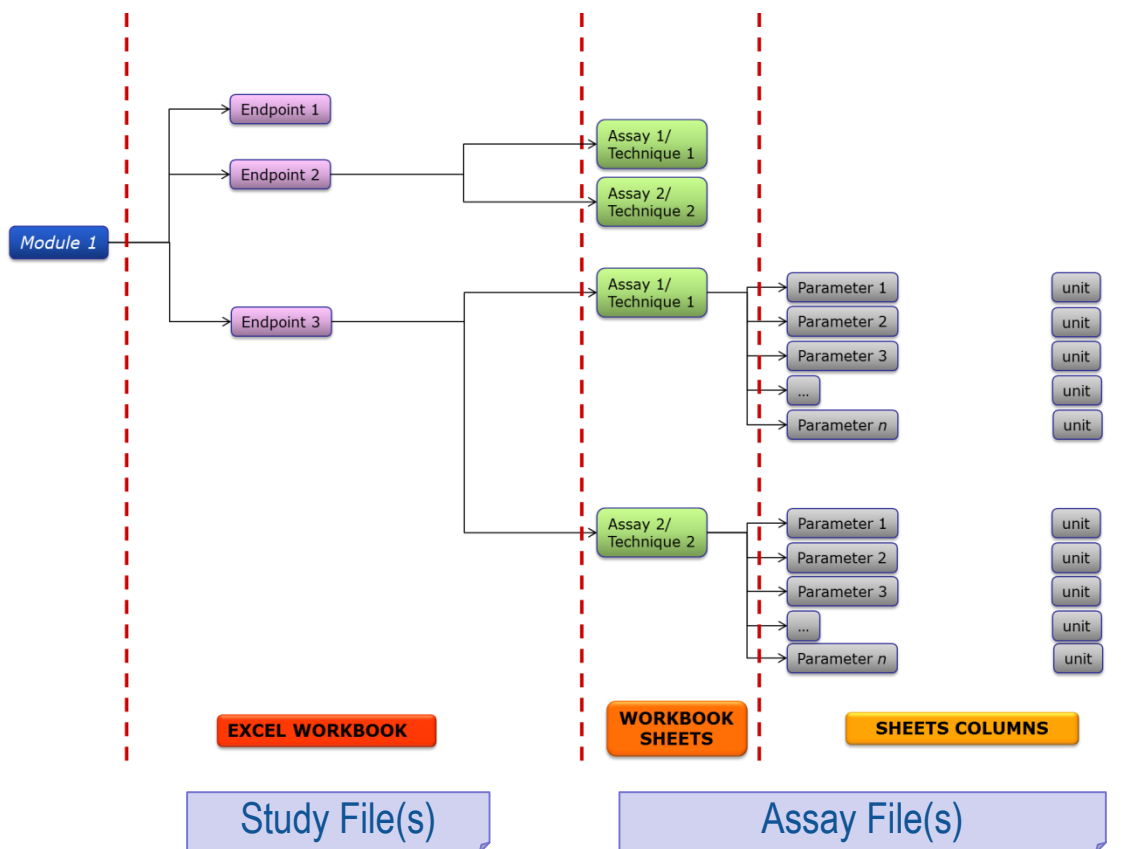Identification of meaningful parameters to describe an assay

Identification of metrics

Inclusion of SOPs

Reproducibility and comparability of logged data

…and the ISA-logic

- Implementation of the ISA-TAB-Nano specification

Way Forward

Public release
of NANoREG templates

→ promoting the harmonisation of data logging to a wider community (beyond NANoREG)

JRC Science Hub
https://ec.europa.eu/jrc

Transfer to a 'central data storage'

→ Translation to the ISA-TAB-Nano specification

View details

Prosafe WP3

Tasks 3.2 and 3.3

Prosafe support to the "data" handling issue
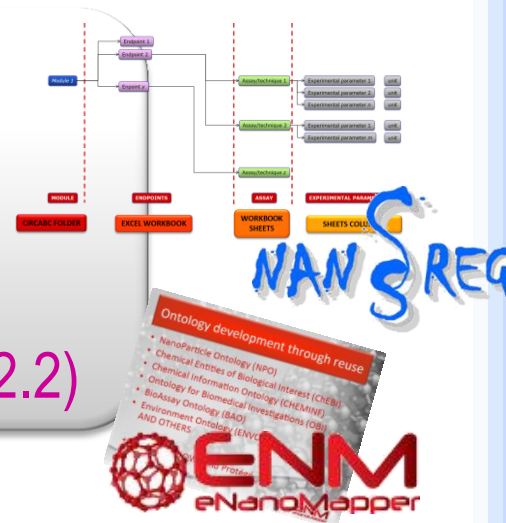
AIMS

Fostering and promoting the harmonisation of data logging via ISA-TAB-Nano (T3.2.1)
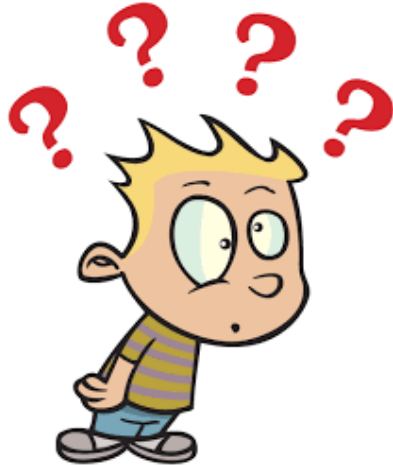
Promoting the eNM ontology (T3.2.2)

ISA-TAB-Nano

RESULTS

Facilitating the use of logged data

Linking approaches and tools in the NSC (T3.3)

Allowing modelling

Facilitating Safe-by-Design (SbD)

Sara.totaro@ec.europa.eu
Hugues.crutzen@ec.europa.eu

Stay in touch

- JRC Science Hub: www.ec.europa.eu/jrc

- Twitter: @EU_ScienceHub

- LinkedIn: european-commission-joint-research-centre

- YouTube: JRC Audiovisuals

- Vimeo: Science@EC