

ProSafe

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Deliverable D 3.3

Minimal ontology and naming convention for nanosafety data

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1 Description of task

From DoW, amended 22.09.2016

Task 3.2.2 - Minimum requirements in ontology and naming conventions – Start M1, end M18
Task Leader: JRC

The ISA-TAB-NANO system development requires also networking among the NanoEHS community and with the Nanosafety Cluster-supporting project eNanoMapper in order to agree upon naming conventions and/or a minimum set of ontology annotations. In that context, the importance of endpoints specific to nanomaterial EHS shall be reviewed.

This sub-task's coordinating work shall take into account the use of OECD harmonised templates (OHTs) and keep in mind the regulatory end format required by REACH, namely IUCLID. Resources, such as OpenToxipedia, shall be carefully reviewed for potential use here, too. This sub-task shall consider the global dimension of the above issues establishing appropriate networking via the PROSAFE global relationships, among others, with standardisation organisations (ISO/CEN), with the CODATAVAMAS working group developing a Uniform Description System for Materials at the Nanoscale (http://www.codata.org/workinggroups/Nanomaterials/Next_Steps.pdf), which is also partner in the recently launched FP7 project FutureNanoNeeds (NMP.2013.1.3-3, www.futurenanoneeds.eu).

2 Description of work & main achievements

2.1 Summary

The intent of gathering a critical mass of adopters in the EU NanoSafety Cluster community around the concept of understanding the need and agreeing to develop a common ontology (coupled with ISA-TAB-Nano) for streamlined data management was successfully supported by this task.

The technical development on ontology development was executed by the FP7 eNanoMapper project, while ProSafe, through this task, has supported the discussions in various arenas, making the audiences aware of the ontology issue, in parallel with the promotion of the ISA-TAB-Nano 'system' (see D3.2).

ProSafe recommends the European Commission to duly consider ways to further integrate the work promoted by ProSafe on data management, ontologies (and ISA-TAB-Nano) in particular, into upcoming strategic nanoEHS R&I funding, and to link this appropriately to the burning issue of data sustainability and curation.

These recommendations of this deliverable and the work on ISA-TAB-Nano serve also as input to the aspects related to data management in the ProSafe White Paper.

2.2 Background of the task

Task 3.2 is divided in two sub-tasks, dealing with two different aspects concerning the creation of a database management system, which i) *ISA-TAB-NANO as backbone for a common database (T3.2.1)* and ii) *Minimum requirements in ontology and naming conventions (T3.2.2)*. The two subtasks are related to two deliverables: i) *D3.2 – ISA-TAB-NANO database system established and adopted within the Nanosafety Cluster*, and ii) *D3.3 – Minimal ontology and naming convention for nanosafety data*.

The general aim of task 3.2 in its whole is the support to the development of a nanoEHS data management system to uniform and follow same conventions when speaking of data reporting

within the EU NanoSafety Cluster. This is also aligned, to a wider extent, with other initiatives that are ongoing e.g. in the US or at OECD level.

This ProSafe sub-task 3.2.2 was setup shortly after the launch of the FP7 project eNanoMapper and linked with it to raise the awareness about the need to develop an appropriate nanomaterials / nanoEHS ontology to enable in Europe a widely-used best practice for flexible data sharing within and among projects (for instance for inter-laboratory comparisons and OECD-level data exchange).

ProSafe, being a Coordination and Support Action, and not a research and innovation one, did not intend to devote efforts to the technical / IT development of ontologies (and the ISA-TAB-Nano system, see D3.2). This was, and is still being done, by other EU-funded projects such as eNanoMapper and H2020 OpenRiskNet.

This task 3.2.2 – of a coordination and support action – is part of an effort to promote the creation of quality-checked datasets, produced by experimentalist (working in separate EU projects) and well-mapped using an adequate and widely-agreed ontology, which can be interlinked and exploited, for instance, by modellers or by regulators.

2.3 Description of the work carried out

While the ProSafe partners of T3.2, in particular JRC, have proposed the adoption of ISA-TAB-Nano for streamlined nanoEHS experimental data recording within the large FP7 project NANoREG, and pushed for its recognition in the EU NanoSafety Cluster (NSC), the leader of this sub-task 3.2.2 underlined within ProSafe the need to simultaneously motivate the NSC towards the adoption of a common 'data description language', i.e. ontology(ies).

Though this need for appropriate nanoEHS/NM ontologies was not a new idea, more needed to be done to get projects to think about how they organise their data (for instance using ISA-TAB-Nano, see D3.2) and, in particular, describe is using 'descriptors'. They should cover the nanosafety domain, encompassing nanomaterials and all information relating to their physicochemical characterisation, as well as relevant experimental paradigms, biological interactions and safety information. These descriptors should be understood, accepted and consistently used by a data-generating nanoEHS community as wide as possible. Indeed, the recognition and comparability of data value thanks to a common ontology greatly enhances the ability to link datasets and, hence, perform data analysis and modelling, which fully exploit the value of those data.

As set in the DoW of T3.2, the task leader has established a strong link with FP7 eNanoMapper right from the start of ProSafe. This has led to a positive collaboration between ProSafe WP3 and eNanoMapper (especially UMaastricht and IDEA) that has lasted for the whole duration of ProSafe. eNanoMapper was the 'technical implementation arm' of a streamlined data management strategy within the EU NanoSafety Cluster (NSC), to serve the data needs of any project in that arena.

In its technical development of ontology for the NSC community, eNanoMapper received support from this ProSafe task 3.2. The task leader relayed on several occasions, such as bilateral JRC-UMaastricht/IDEA teleconferences, participation in eNM-promoted NSC meetings in 2016, monthly TC calls of the NanoSafety Cluster WG4 US-EU CoR meetings on databases, etc. the needs of the nanoEHS community, especially of the large project NANoREG via the public release by JRC of the NANoREG templates¹.

¹ Totaro S. et al; Data logging templates for the environmental, health and safety assessment of nanomaterials; EUR 28137 EN; doi:[10.2787/505397](https://doi.org/10.2787/505397); January 2017

eNanoMapper's defining work on ontologies for the NSC (and beyond) has been published in detailed technical deliverables²³⁴.

2.4 Results

The intent of gathering a critical mass of adopters in the EU NanoSafety Cluster community around the concept of understanding the need and agreeing to develop a common ontology (coupled with ISA-TAB-Nano) for streamlined data management was successfully supported by this task.

The technical development was executed by the eNanoMapper project, as reported in their deliverables D2.1, D2.2 and D2.3 (see ref. in section 5). As written in D2.1, "*the ontology is being developed in the Web Ontology Language (OWL: W3C, 2012). OWL is a standard approved by the W3C for the representation of domain knowledge embedded in a semantic web framework. It is increasingly being adopted by the life sciences community for their ontology development efforts, and the provision of multiple ontologies in the same underlying language aids interoperability and convergence to a common framework.*"

This has been a good example of cross-project collaboration: Coordination and Support with Research and Innovation.

The ISA-TAB-Nano 'system' coupled with the developed, yet still evolving, ontology is now a reality that has enabled the creation of first NSC project databases that become searchable and linkable, e.g. the NANoREG-eNanoMapper database: <https://search.data.enanomapper.net/nanoreg/>. New initiatives (and existing ones) in the NSC and the European Commission, as funder, inevitably have to consider its usefulness for full exploitation of datasets generated in nanoEHS using, among others, large amounts of public funding.

2.5 Evaluation and conclusions

This ProSafe work in WP3 to find a way to deploy a streamlined data management strategy by combining ISA-TAB-Nano with adequate nanoEHS ontology has proven useful and has attracted the attention of and stimulated on-going collaboration in the NSC and with the US, in particular with Duke University, which has been linked to ProSafe in WP1.

Ontology development is a rather complex field of activity and easily leads to intricate metadata management systems. Key to the success should always be keeping the system as simple as possible. Thanks to the expertise found in eNanoMapper, a widely agreeable ontology based on OWL (see eNanoMapper deliverable D2.1 – ref. in section 5), is being realised in for the NSC.

ProSafe recommends the European Commission to duly consider ways to further integrate the work promoted by ProSafe on data management, ontologies and ISA-TAB-Nano in particular, into upcoming strategic nanoEHS R&I funding, and to link this appropriately to the burning issue of data sustainability and curation.

These recommendations of this deliverable and the work on ISA-TAB-Nano serve also as input to the aspects related to data management in the ProSafe White Paper.

² Janna Hastings, Gareth Owen, Egon Willighagen, Barry Hardy. Deliverable Report D2.2 Ontology Content Types and Existing Community efforts. (Zenodo, 2014). doi:10.5281/zenodo.375634

³ Janna Hastings, Egon Willighagen, Barry Hardy. Deliverable Report D2.1 Framework and Infrastructure for Ontology development, versioning and dissemination. (Zenodo, 2014). doi:10.5281/zenodo.375633

⁴ Janna Hastings, Egon Willighagen, Gareth Owen, Barry Hardy. Deliverable Report D2.3 Ontology initial release. (Zenodo, 2015). doi:10.5281/zenodo.375635

3 Deviations from the work plan

The effort in T3.2.2 started about a year later than foreseen, since the efforts of its leader were very focused on the ISA-TAB-Nano aspects (T3.2.1) and the successful mapping of existing databases (T3.1). However, this delay did not impact the rest of the project and the good collaboration between the task leader and eNanoMapper has been beneficial.

4 Performance of the partners

The partner performed adequately.

5 References / Selected sources of information (optional)

Totaro S. et al; Data logging templates for the environmental, health and safety assessment of nanomaterials; EUR 28137 EN; doi:[10.2787/505397](https://doi.org/10.2787/505397); January 2017

Janna Hastings, Gareth Owen, Egon Willighagen, Barry Hardy. Deliverable Report D2.2 Ontology Content Types and Existing Community efforts. (Zenodo, 2014). doi:10.5281/zenodo.375634

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