

Database WG

U.S.-EU NanoEHS Workshop, Arlington, Dec 2-3 2013, #USEUnanoEHS

Egon Willighagen (on behalf...)
Maastricht University, The Netherlands

@egonwillighagen ORCID:0000-0001-7542-0286

Access Point

Our homepage:

http://www.nanosafetycluster.eu/working-groups/4-database-wg.html

or: http://goo.gl/RliQO2

NSC WG4 homepage

Database WG



Databases working group

Chair: Egon Willighagen, Maastricht University (eNanoMapper, ORCID: 0000-0001-7542-0286)

Co-Chair: Iseult Lynch, University College Dublin (NanoTransKinetics, QNano, NeuroNano)

The Databases WG of the EU Nanosafety Cluster is tasked with agreeing on data interoperability and a common language (one or more ontologies) for European databases for project results and data, that will ensure longevity of data (beyond individual project lifetimes) and enable wide uptake and accessibility of the data to modellers, risk assessors and other researchers, as well as being able to communicate with other international databases.

The first step towards this is an assessment of the current state-of-the-art in available databases and nano-etymology, to ensure that we are not reinventing the wheel, but that our decisions are informed, and our final product meets the needs of the entire research community.



Participation

Monthly teleconferences are organized on the second Tuesday of the month, at 3pm CEST (or 3pm CET). Please also register your interest to participate by joining the mailing list.



Connections

This working group is in contact the <u>US-EU Community of Research</u> and the US <u>Nano WG</u>.



Minutes and Telcon Transcripts

participants.html

Participants



In alphabetic order (email the WG4 mailing list with details if you like to be added to this list):

Name (Institute)	NSC Project(s)	WG4 Tasks	Interests
Christoffer Åberg (University College Dublin)	NanoTransKinetics	<u>2013-2</u>	Modelling of nanoparticle-cell interactions
David Carlander (Nanotechnology Industries Association)	MARINA, NanoEIS, NanoLyse, NANoREG, Scaffold		Risk assessment, legislation, regulatory toxicity, applications, innovation, SME support
Barry Hardy (DouglasConnect)	eNanoMapper		
Sonja Hartl (BioNanoNet Forschungsgesellschaft mbH)	NANoREG		Regulatory and Standardization Aspects of ENM; Risk assessment, Toxicity; Innovation, Communication & Dissemination
Nina Jeliazkova	eNanoMapper		databases, ontologies, APIs, prediction, toxicology, QSAR
Richard Marchese Robinson (Liverpool John Moores University)	NanoPUZZLES		chemoinformatics, QSAR, data models,
Axel P. Mustad (NQCG)	MARINA, NANoREG	<u>2013-1</u>	Ontology learning, Databases, Semantic Web Technologies, Nanotechnology, Standardisation, e- Infrastructures.

Project Ideas (mutable)

Project Ideas



Idea: Limitations of ISATab-Nano and the NanoParticle Ontology

Contact: ?

Description: The WG4 has expressed interest in adopting the ISATab-Nano and NPO standards. At the same time it is acknowledge that the current version may not accommodate for all NSC use cases. It therefore like to explore and document such limitations to support future development and/or contributions to these standards.

Idea: Target Audience

Contact: ?

Description: Databases support users of various kinds. The WG4 should explore the various users that the WG4 should service.

Idea: End Points

Contact: ?

Description: Make an ontology of end points relevant to NSC research, allowing linking of studies. The BioAssay Ontology may be useful here.

Idea: Database Identifier Mappings

Contact: ?

Description: Various databases have information and experimental data on nanomaterials. Where possible links between the same nanomaterial in different databases should be made, using identifier mappings.

Idea:

Contact: ?

Task 1:







Updated list of (NSC) Databases

Contact: Axel P. Mustad, Nordic Quantum Computing Group AS (NQCG) mailing list

Not too long ago a list of nanosafety-related databases have been composed, but in a fast-pacing world this lists need maintenance. Additionally, the list should be completed with further detail on these databases, including whether the database has an API, uses standards (e.g., ontologies), and what the copyright and license state is.

Contributing: Egon Willighagen, ... (please let Axel P. Mustad know you would like to participate).

Working draft:

Note: This is a work in progress, and should not be seen as the unaminous final recommendation of WG4, but merely a suggestion to be discussed.

Development of a matrix with features of the databases (see mailing list). The matrix is intended to help administrators of nanosafety related databases to broaden awareness of their databases and to ensure interoperability of data from multitude databases worldwide.

- Instance or schema data
 - · Does data store hold instance or schema data or both?
- · Instance data: structured or unstructured
 - Is instance data structured, e.g., relational, unstructured texts, or both
- · Data description
 - Describe data contents
 - Name important classes, properties (in case of schema data)
 - Informally describe instances (in case of instances data)

Task 2







Overview and recommendation of data quality

Contact: Christoffer Åberg, University College Dublin (NanoTransKinetics)

The WG4 will document and keep accurate a working definition of data quality and recommend a minimal standard for reporting.

Working draft

Note: This is a work in progress, and should not be seen as the unaminous final recommendation of WG4, but merely a suggestion to be discussed.

- nanoparticle
 - chemical composition
 - crystal structure/crystallinity
 - purity
 - shape (incl. aspect ratio etc)
 - o surface area
 - surface charge
 - surface chemistry (including composition and reactivity)
 - solubility
- · dispersion medium
 - medium
 - o concentration of serum
 - origin of serum (species)
 - heat treatment

Monthly conference calls

Second Tuesday of the month, 15 CEST/CET



Minutes and Telcon Transcripts

- 2013-12-10 monthly telcon
- 2013-12-02/03 2013 U.S.-EU NanoEHS Workshop
- 2013-11-20 (delayed) monthly telcon
- 2013-10-08 monthly telcon
- 2013-09-20 WG4 breakout in Birmingham
- 2013-09-10 telcon (transcript)
- 2012-03-01 WG4 Meeting Dublin

Join!

Sign up to the Database WG mailing list:

http://nanosafetycluster.eu/mailman/listinfo/wg4-database

Info about the **EU NanoSafety Cluster** (@EUNanoSafety):

http://www.nanosafetycluster.eu/home/subscribe-to-newsletter.html