Nanosafety databases: harmonisation efforts in Europe

Iseult Lynch & Teresa Fernandes

EU NanoSafety Cluster WG4

NanoSafety Cluster

SEVENTH FRAMEWORK PROGRAMME

Objective of NSC WG4

To develop an EU-project-wide strategy for capturing and storing data emerging from EU-funded projects, thereby reducing the duplication of costs / effort in EU-funded projects for data management.

- Not a trivial task. Need to address issues around:
  - Descriptors for all aspects of materials, characterisation, impacts (tox & ecotox), exposure, LCA, modelling, QSARs etc.
  - Capture negative and positive effects
  - Data input & Quality assurance
  - IPR & data confidentiality issues
  - Design, implementation and maintenance strategies & PM
  - Build on existing best practice, be adaptable to new developments in science & regulation

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- Teresa Fernandes
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- Rafi Korenstein (NHECD)
- Claus Svedsson (NanoFate)
- Hubert Rauscher (NanoHub)
- Stacey Harper
- All NanoSafety Cluster WG4 members

2013 – 2 new projects

NMP.2013.1.3-2 Nanomaterials safety assessment: **Ontology**, **database(s)** for modelling and risk assessment

NMP.2013.1.3-3 Development of a systematic framework for **naming** and assessing **safety** of the **next generations** of nanomaterials being developed for **industrial applications**

=> Specific budget for this task, but must serve needs of the research community, i.e. the NSC members are a primary stakeholder

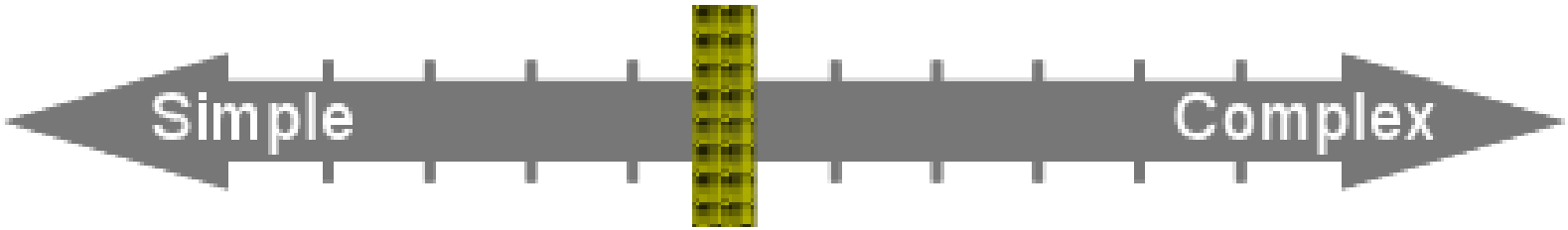
Unique Opportunity for Nanosafety Community

- **Gather, manage interpret current and future research**
  - Research typically 5-10 years ahead of regulation
  - Complex, unstructured data
    - properly addressed will point to broad rules for nanosafety evaluation / regulation,
    - poorly managed, lost for a decade, lost investment

- **Move Nanosafety research beyond legacy nanomaterials**
  - New complex shapes / architectures – how to describe these?
  - Radically new materials: core, shell, functionalisation & *context* matter

How much to harmonise?

Which level of harmonisation is „just right“?



Too simple:

- identified requirements cannot be supported
- insufficient harmonisation
- few benefits

Too complex:

- difficult to implement
- substantial benefits available only to few users
- high cost

Optimal database format

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- For a functional and usable database there are three perspectives:
  - bench researcher,
  - modeller,
  - enterprise needs such as regulation.

- Need sufficient flexibility so that emerging / undiscovered end-points can be captured

- Need to capture exposure context & transformations

Usability for researchers

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- Data entry should be real-time
  - E.g. electronic notebook integration
  - This will ensure that *negative data* (i.e. where no effect is observed) is also captured

- Raw data files / qualitative information & not just the excel analysis (quantitative information)
  - for modelling & additional data extraction)
  - additional flexibility – e.g. conversion to other metrics
  - enable re-analysis of data for new purposes

Issues around data sharing

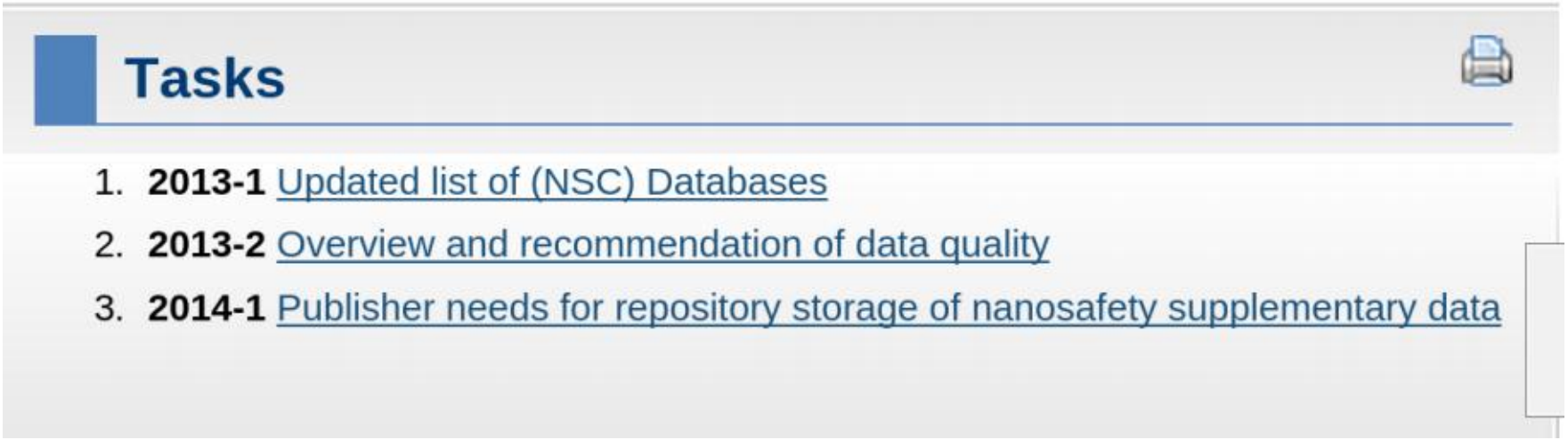
- What will incentive researchers to share their data?
- Can we made the database citable & acknowledge contributors / funding sources?
- Can we agree guidelines for authorship / acknowledgement for work on “shared” datasets?
- Can we get publishers to support data sharing? E.g. proteomics and crystallography communities

WG4 Re-launched Sept 2013

- NSC meeting Sept 2013 Birmingham
- All WGs defined short, medium & long term goals
- Driven primarily since Sept 2013 by Egon Willighagen (eNanomapper) and Richard Marchese Robinson (NanoPUZZELS)

Community Building

- regular monthly telcons
  - typically 5-10 people on the call
- three joint tasks
- 91 people on the mailing list



Database Survey Results

Summary of the Spring 2014 NSC Database Survey

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Abstract

The NanoSafety Cluster Database working group organized in Spring 2014 a survey for the community to summarize the current state of databases and including questions of a more

- What did the survey ask?
- 1. general info (website, owners, …)
- 2. type of content
- 3. how can data be looked at
- a. HTML, PDF, Excel, …
- 4. Application Programming Interfaces (APIs)
- a. REST, SOAP, …
- b. Format standards
- 5. Semantics
- a. ontologies, …

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    b. Format standards
5. Semantics
    - a. ontologies, …
6. Licensing
    - a. is the licensing clearly stated?