NanoSafety Cluster WG4: databases

Birmingham, 2013-09-20. Minutes by Pekka.

Participants: Egon Willighagen (Chair, presenter), Person 1 (German Company), Michaela Pettit (ModNanoTox, presenter), Christoffer Åberg (UCD, presenter), Janna Hastings (EBI), Pekka Kohonen (KI), Richard Marchese Robinson (data collection and database design. Extracting data from the literature. Transfer and collection into standards. Relational databases and semantic web ontologies), Valsami-Jones: ModNanoTox, databases + coordinator of NanoMILE.

Presentation: ModNanoTox, Michaela Pettit.

Modeling toxicity of ENS at multiple levels. WP1 atomistic modelling. WP3 classical toxicological studies: uptake/bioaccumulation, WP6 population modelling and risk assessments, WP2 extraction and validation / evaluation of data (not DB building*),

partners: University of Birmingham, In silico technology SME (also in eNanoMapper), Univ. Nebraska (US-collab), ...

Issues: not able to get any unpublished data to put on the DB, take note of sister studies (one part in one paper, other in other paper), Commercially done NPs are of a lower quality?,

DB: ModAtlas, Structure: 4 fields (DB tables, not-relational, tabular): bibliographic, particle characteristics, assay details, study outcomes.

Data gaps: characterization in situ not as good as should be (improving) e.g. characterize what the organism is actually exposed to. Endpoint gaps: uptake/depuration data with temporal components/ kinetic data.

Data types: tabulated, graphical data (digitized graphs and extract data), evaluation important, low benchmark for inclusion into DB, score for completeness of material characterization (material dependent)

Models: population, QSAR, atomistic, bioaccumulation, ...

Data corpus: 90 studies, mainly silver, # of particles?

Janna will contact IST (David Vorg) to talk about ontologies used in the ISA-Tab-Nano conversion of the Excel-based ModNanoTox data.

Lessons: make fields as specific as possible, define fields precisely, do not assume it is correct because is published, Experimentalists: make sure to include details that are most critical for biological data interpretation (many studies missing critical information), should be a

“minimal-”minimal information standard.

NOTE: ModNanoToxDB converted to ISA-TAB-Nano by In Silico/UoB for use in eNanoMapper

NanoWG Note: quantifying statistics, statistics (what percentage of papers characterize large # of particles for small # of endpoints, and visa-versa)

WG4 work idea: write a review paper about the quality of

Presentation: NanoTransKinetics, Christoffer Åberg (UCD).

Nutshell: location of action drives toxicity: models spatial kinetics (e.g. spatial, intracellular location of NPs), interactions with cell membrane, transport inside cells, passage through barriers,

WP1: Data acquisition and QC, WP5 integration and software tools

Lessons: dispersion characteristics e.g. EM images, is the study looking at single particles or agglomerates (changes as a function of time);

corona concept/interactions with biological fluid constituents/biomolecules: first contact with biological fluid (e.g. lung surfactant, gut fluid, blood plasma), testing the toxicity of corona-covered NPs, actually. can have effects on: toxicity, uptake, escape into the cytosol (often particles w/o corona are more toxic e.g. interaction energy reduced by corona)

Issues: corona, even different media can have large effects on toxicity; heat inactivation: complement of the serum can be inactivated by heat, changes uptake -> normal serum has much higher uptake, than complement-free heat inactivated serum

Issues (state of the cells): cell density changes uptake - influence on toxicity (J.A Kim et al. Nat. NanoTech 7, 62-68, 2012); G2/M phase cells have higher amount of NPs; G0 cell least uptake (in vivo), Cell preparation: different amount uptaken dependent on preparation (different toxicity) Åberg et al. Europhysics Letters 1012, 38007, (2013); Solutions: describe study very well (size of dish, time)

Issues(particle source): number of NPs must be large enough to cause potential toxicity, volumes and supply not reported

Issues(NP amounts): is the NP amount enough to actually caused toxicity, often only concentration reported and not the volume the cells and NPs suspended in.

Corona formation speed : so rapid that never see the ”naked” particle. Will acquire corona from somewhere else. Naked particles, corona is composed of cytosol components (pierced cells),

Biological identity of particle to perform matching, and read-across. How to define standard conditions for measuring the corona.

Janna: structural formats for nanostructures, is it possible. Extend ideas from other fields

Discussion on database design:

limit discussion to problems that can be solved by available data (expanding scope as data increases)

manpower is a limiting factor in DB construction

future-proofing database design,

ISA-TAB-nano:

- Format does not define what included
- Ontology (NPO) should support definition of types of measurements want to record
- Remit not to define what should record but enable recording
- Minimum content check-list
- Tools to validate syntax
- Baker: coordinate usage of ISA-TAB-nano, ISA-tools, working to revise format, so that software left as is, used with guidelines to validate/create isatab files
- NPO: is it designed on yesterday's data,
- Keeping track of what matters: and including that

Presentation eNanoMapper

eNanoMapper partners: DouglasConnect, Switserland; Nat. Tech. Univ. of Athens, Greece; In Silico Technologies, Switserland; IdeaConsult Ltd., Bulgaria; Karolinska Institutet, Sweden; VTT Technical Research Center of Finland; EMBL-EBI, UK; Maastricht University, The Netherlands

Connections: NMP2013-1.3-3 (naming of nanomaterials), CENELEC, NanoWG, publishing industry, NIA, associate partner program.

Role:

- How much WG4 and eNanoMapper priorities and tasks overlap?
- Platform to support proprietary data (security protocols)
- Not develop a monolithic solution but use linked data and interoperable solutions
- Softwares used: OpenTox framework, AMBIT, ISA-tools, other open source tools as

required

- Ontologies: ISATab, NPO, CHEMINF, BioAssay Ontology, QUDT, …

OpenTox meeting 30.9-2.10, http://www.opentox.org/meet/opentoxeu2013

eNanoMapper calls:

- Call is the result of this WG4: NMP2013-1.3-2.
    - API needed

Minutes: Projects Ideas

- DB review: API available, ontologies involved?
- Review paper on the badness of literature
- Existing db and ontology mapping
- Defining minimum information standards
    - Should not independently create standards
    - Stakeholders ask them now
    - Aggregate list of standards and keep it
    - NanoMine: list of attributers contribute
    - Chat: capture information standard already?