

eNanoMapper Resources & Interactions

Data, Ontology and Harmonisation Needs for Nano Safety Cluster & Projects, 25 January 2016, Brussels

Barry Hardy, Douglas Connect GmbH
Project Coordinator



Meeting Agenda

Time	Topic	Responsible
09:30 - 09:45	Introduction and Objectives	Georgios Katalagarianakis and Nicolas Segebarth (EC)
09:45 - 10:15	eNanoMapper Resources & Interactions	Barry Hardy (Douglas Connect)
10:15 - 11:15	Harmonisation, Ontology & Templates	Egon Willighagen (Univ. Maastricht)
11:15 - 11:30	Coffee Break	
11:30 - 12:30	Data Management	Nina Jeliazkova (Ideaconsult)
12:30 - 13:15	Lunch break	
13:15 - 14:30	Applications and Project Needs	Roland Grafstrom (Karolinska Institute) and Iseult Lynch (University of Birmingham)
14:30 - 16:00	Cluster Needs, Impact and Sustainability	Barry Hardy (Douglas Connect) and Peter Ritchie (Institute of Occupational Medicine)
16:00 - 16:30	Conclusions	Georgios Katalagarianakis and Nicolas Segebarth (EC)



Main objectives of eNanoMapper

- Modular infrastructure for **data storage, sharing and searching**, based on **open standards** and semantic web technologies, minimum information standards and established **security** solutions
- Development of **ontologies** for the categorisation and characterisation of Engineered Nanomaterials (ENMs) in collaboration with other projects
- Creation of new computational models in nanomaterials safety through the implementation of interfaces for **toxicity modelling and prediction** algorithms which may process all data made available through eNanoMapper (e.g. using algorithms available from the OpenTox project or statistical/data mining software)
- **Meta analysis of nano-bio interactions** supporting “safe-by-design” ENMs development by pursuing a Linked Data approach which integrates data and metadata originating from diverse sources within nanoscience, chemistry, biology and toxicology
- Creation of **tools** for the exchange, quality assurance and reporting of research protocols and data for regulatory purposes
- Creation of a **community** framework for interdisciplinary collaboration



OpenTox and Open Components and Standards

<-New API addition from ToxBank

Investigation (Study, Assay)

GET
POST
PUT
DELETE

Authorisation & Authentication

GET
POST
PUT
DELETE

AppDomain

GET
POST
PUT
DELETE

Report

GET
POST
PUT
DELETE

Dataset

GET
POST
PUT
DELETE

Validation

GET
POST
PUT
DELETE

Feature

GET
POST
PUT
DELETE

Compound

GET
POST
PUT
DELETE

Model

GET
POST
PUT
DELETE

Ontology

GET
POST
PUT
DELETE

Algorithm

GET
POST
PUT
DELETE

OpenTox and Sustainability



HOME

RESOURCES

LIBRARY

EVENTS

OPENTOX ASSOCIATION

ABOUT

**OUR FRAMEWORK
PROVIDES TOOLS
FOR DATA INTEGRATION**



**Working Group Discussions on
Data, AOPs, APIs to incorporate
eNanoMapper extensions**

www.opentox.net

ToxBank and Sustainability



- 1) Sustaining as an OpenTox Reference Resource
- 2) Developing further within Second Phase (EUToxRISK)
- 3) Commercialising through ToxHQ

HOME

PUBLIC FORUM

RESOURCES

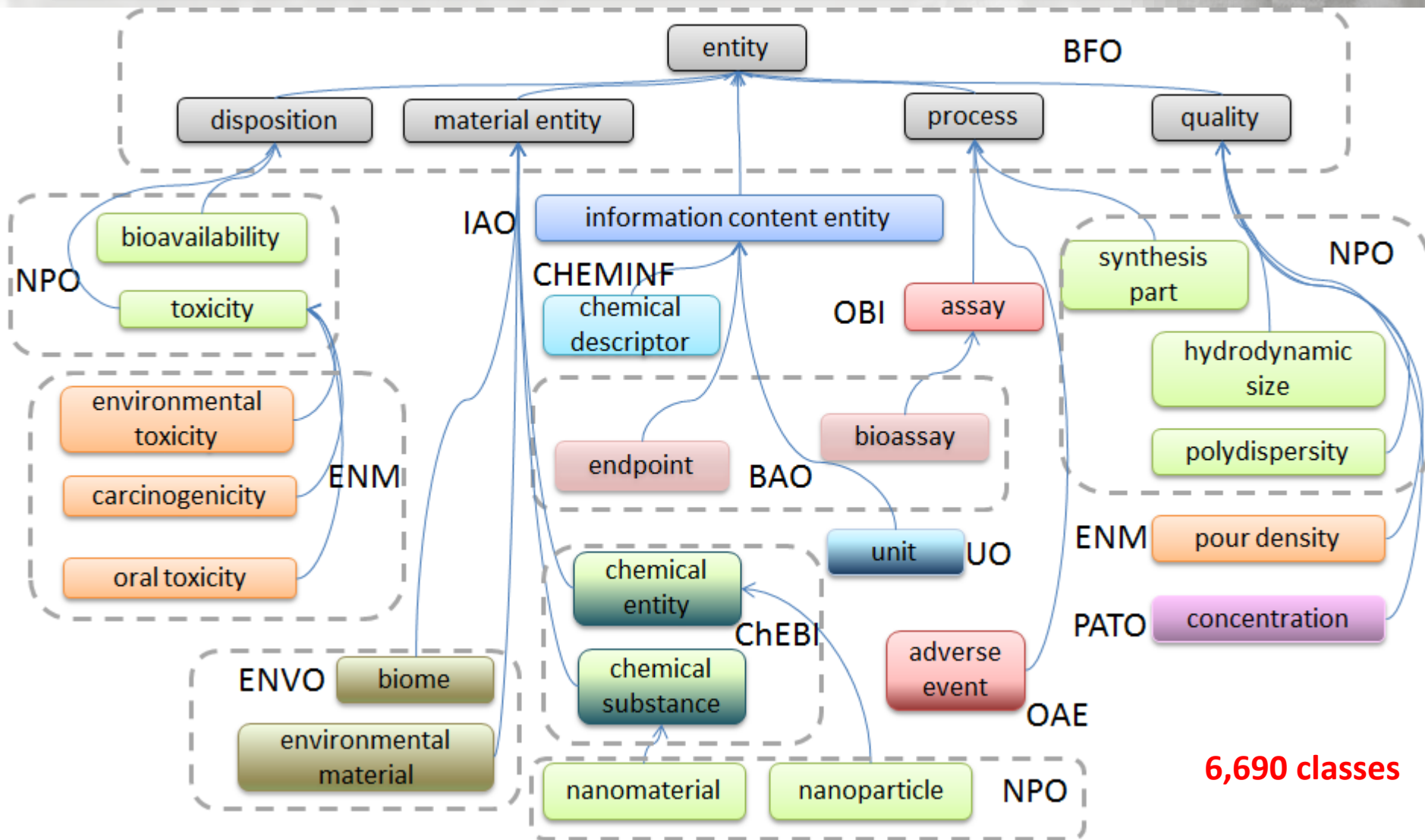
LIBRARY

DEVELOPMENT

ABOUT

**SUPPORTING
INTEGRATED
DATA ANALYSIS**

Ontology assembled from multiple sources



eNanoMapper Ontology in Protegé

Open in Protegé purl.enanomapper.org/onto/enanomapper.owl

The screenshot displays the Protegé web interface for the eNanoMapper ontology. The browser address bar shows the URL <http://purl.enanomapper.org/onto/enanomapper.owl>. The interface includes a navigation menu with options like Active Ontology, Entities, Classes, Object Properties, Data Properties, Annotation Properties, Individuals, OWLViz, DL Query, OntoGraf, SPARQL Query, and Ontology Differences. The main content area is divided into several sections:

- Ontology header:** Contains the Ontology IRI (<http://purl.enanomapper.org/onto/enanomapper.owl>) and the Ontology Version IRI (e.g., <http://purl.enanomapper.org/onto/enanomapper.owl/1.0.0>).
- Annotations:** A list of annotations with expand/collapse icons. The annotations include:
 - Contributor:** Nina Jeliazkova
 - comment:** The eNanoMapper project (www.enanomapper.net) is creating a pan-European computational infrastructure for toxicological data management for ENMs, based on semantic web standards and ontologies. This ontology is an application ontology targeting the full domain of nanomaterial safety assessment. It re-uses several other ontologies including the NPO, CHEMINF, ChEBI, and ENVO.
 - license:** CC-BY 3.0 <https://creativecommons.org/licenses/by/3.0/>
 - Contributor:** Gareth Owen
 - Contributor:** Ianna Hastings
- Ontology metrics:** A table showing metrics for the ontology.
- Imported ontologies:** A section for listing imported ontologies, with sub-sections for Ontology imports, Ontology Prefixes, and General class axioms.

Metrics	
Axiom	48483
Logical axiom count	5910

REST Application Programming Interface

API documentation (Swagger-UI)

The screenshot shows the Swagger-UI interface for the eNanoMapper API. At the top, there is a header with the ENM logo, a search bar containing 'api_key', and an 'Explore' button. Below the header, the main content area is titled 'eNanoMapper prototype database API' and includes a description: 'AMBIT REST web services 2.7.2 (with enanmapper profile). More at <https://apps.ideaconsult.net/enanmapper>'. There are links for 'Terms of service', 'Contact the developer', and 'License'. A list of services follows, each with a name and a 'Raw' link: 'algorithm : OpenTox Algorithms service', 'bundle : Datasets of substances', 'compound : OpenTox Chemical Compounds service', 'dataset : OpenTox Dataset service', 'feature : OpenTox Feature service', 'model : OpenTox Prediction Models service', 'property : Chemical substances Properties service', 'query : Queries', 'compound : Chemical structures search', 'substance : Substance search', 'substance : Chemical Substances service', 'substanceowner : Substance owners', and 'task : OpenTox Task service (asynchronous jobs)'. The 'substance : Chemical Substances service' is expanded, showing a list of endpoints: GET /substance (List substances), POST /substance (Import substance(s) and studies), GET /substance/{uuid} (Get a substance), GET /substance/{uuid}/composition (Get substance composition), GET /substance/{uuid}/structures (Get substance composition as a dataset), GET /substance/{uuid}/study (Get substance study), and GET /substance/{uuid}/studysummary (Get study summary for the substance). At the bottom, the base URL is given as 'https://apps.ideaconsult.net/enanmapper/api-docs' and the API version as '2.7.2'.

Interactive API queries

The screenshot shows the interactive API query interface for the 'substance : Chemical Substances service'. The top bar includes 'Show/Hide', 'List Operations', 'Expand Operations', and 'Raw'. Below this, a list of endpoints is shown, with the 'GET /substance/{uuid}/study' endpoint selected. The interface displays the 'Implementation Notes' for this endpoint, which is 'Substance study'. The 'Response Class' is 'Model' and the 'Model Schema' is shown in a yellow box with a scroll bar. The schema is a JSON object with the following structure:

```
{  "interpretation": "object",  "name": "object",  "parameters": "object",  "protocol": "object",  "reliability": "object",  "units": ""}
```

 Below the schema, the 'Response Content Type' is set to 'application/json'. The 'Parameters' section is a table with columns for 'Parameter', 'Value', 'Description', and 'Parameter Type'. The parameters are: 'uuid' (value: 'NWKL-02981d44-b7d0-34c8-abab-dd19a5a40865', description: 'Substance UUID', type: 'string'), 'top' (value: 'P-CHEM', description: 'Top endpoint category', type: 'string'), 'category' (description: 'Endpoint category (the value in the protocol category code field)', type: 'string'), 'property' (description: 'Property UUID', type: 'string'), and 'property_url' (description: 'Property URI https://apps.ideaconsult.net/enanmapper/property/{UUID} , see Property service', type: 'string'). There are also input fields for 'page' (value: 0) and 'pagesize' (value: 10). The 'Response Messages' section is a table with columns for 'HTTP Status Code', 'Reason', and 'Response Model'. The messages are: 200 (OK), 400 (Invalid substance identifier), 404 (Substance not found), 403 (Forbidden), 401 (Not Authorized), 405 (Method not allowed), 500 (Internal server error), 501 (Not implemented), and 503 (Service unavailable). The 'Request URL' is shown as 'https://apps.ideaconsult.net:443/enanmapper/substance/NWKL-02981d44-b7d0-34c8-abab-dd19a5a40865/study?top=P-CHEM&page=0&pagesize=10'. The 'Response Body' is shown in a yellow box with a scroll bar, containing a JSON object:

```
{  "TEST_RESULT_FORM": null,  "reliability": {    "is_substudy": "false",    "is_used_for_classification": "false",    "is_used_for_nomenclature": "false",    "purpose": "null",    "study_result_type": "experimental_result",    "value": "null"  },  "interpretation": {    "result": "null"  },  "effects": [    {      "endpoint": "PARTICLE SIZE",      "conditions": {},      "result": {        "unit": "nm",        "invalue": 20      }    }  ]}
```

<http://enanomapper.github.io/API/>



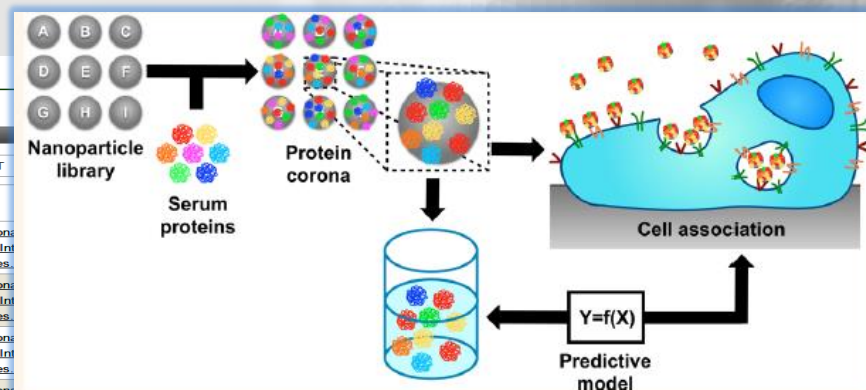
Prototype database (NM components)

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search substances by identifiers

Showing from 1 to 100 in pages of 100 substances

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID		
- 11 -	G15.DDT@BDHDA	FCSV-2a853f39-4...	nanoparticle	G15.DDT@BDHDA	FCSV-2a853f39-4...	Protein Corona the Cellular Int Nanoparticles.csv
- 12 -	G15.DDT@CTAB	FCSV-d1731b11-2...	nanoparticle	G15.DDT@CTAB	FCSV-d1731b11-2...	Protein Corona the Cellular Int Nanoparticles.csv
- 13 -	G15.DDT@DOTAP	FCSV-3b96ad7a-b...	nanoparticle	G15.DDT@DOTAP	FCSV-3b96ad7a-b...	Protein Corona the Cellular Int Nanoparticles.csv
- 14 -	G15.DDT@ODA	FCSV-fb5e6048-8...	nanoparticle	G15.DDT@ODA	FCSV-fb5e6048-8...	Protein Corona the Cellular Interaction of Gold and Silver Nanoparticles.csv

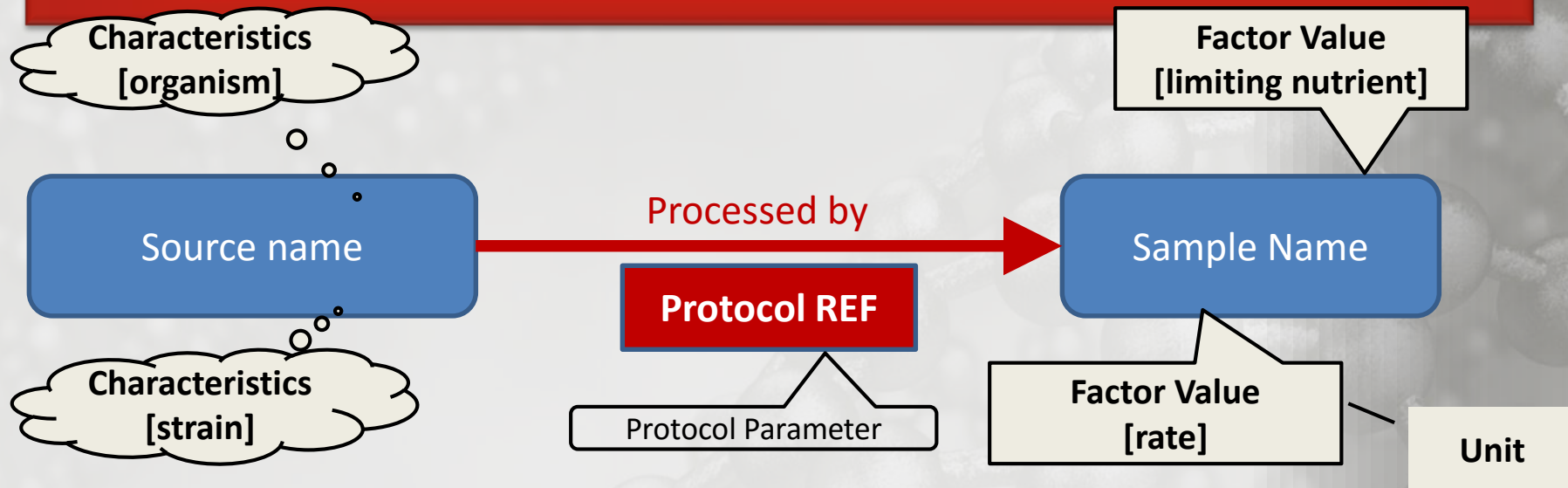


Protein Corona Data set
DOI:10.1021/nn406018q

Composition name: FCSV-fb5e6048-8ee1-351d-915b-d1669681357e
Composition UUID: FCSV-fb5e6048-8ee1-351d-915b-d1669681357e
Purity of IUC Substance:


Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Coating	Dodecane-1-Thiol,Wnahlzmsdqwp-Uhfffoaoya-N.Inchi=1s/C12h26s/C1-2-3-4-5-6-7-8-9-10-11-12-13/H13h,2-12h2,1h3,1-Dodecanethiol			0 % (w/w)	0 % (w/w) 0 % (w/w)	Also contained
Coating	Octadecan-1-Amine,Reyjpvsyryzge-Uhfffoaoya-N.Inchi=1s/C18h39n/C1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/H2-19h2,1h3,Stearylamine,1-Octadecanamine,Octadecylamine			0 % (w/w)	0 % (w/w) 0 % (w/w)	Also contained
Core	[Au]			0 % (w/w)	0 % (w/w) 0 % (w/w)	Au

- 15 -	G15.DDT@SA	FCSV-cd7105f2-f...	nanoparticle	G15.DDT@SA	FCSV-cd7105f2-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic
- 16 -	G15.DDT@SDS	FCSV-9505d90b-f...	nanoparticle	G15.DDT@SDS	FCSV-9505d90b-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic
- 68 -	G30.DDT@BDHDA	FCSV-50aee86c-a...	nanoparticle	G30.DDT@BDHDA	FCSV-50aee86c-a...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic
- 69 -	G30.DDT@CTAB	FCSV-c4e9df58-f...	nanoparticle	G30.DDT@CTAB	FCSV-c4e9df58-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic



Source Name	Characteristics [organism]	Characteristics [strain]	Protocol REF	Sample Name	Factor Value [limiting nutrient]	Factor Value [rate]	Unit
culture1	Saccharomyces cerevisiae	FY1679	growth protocol	C-0.07-aliquot1	carbon	0.07	l/hour
culture4	Saccharomyces cerevisiae	FY1679	growth protocol	N-0.07-aliquot1	nitrogen	0.07	l/hour
culture5	Saccharomyces cerevisiae	FY1679	growth protocol	N-0.1-aliquot1	nitrogen	0.1	l/hour

Protocol service


Protocol User management ▾ Admin ▾ Help ▾
[nina] Log out

Protocols


Showing 15 protocols (1 to 10)

Identifier	Title	Status / Owner	Abstract	Project	Organisation	Updated
ENMNSC-Protocol-1-1	Comet Assay <small>Published: Yes</small> Download	RESEARCH Owner	This protocol describes the single cell gel electrophoresis assay (also known as the Comet assay) which is a simple, rapid and sensitive technique for analysing and quantifying DNA damage in individual mammalian (and to some extent prokaryotic) cells. This was first introduced by Ostling and Johanson in 1984. This was a neutral assay in which the lysis and electrophoresis were done under neutral conditions. Staining was done with acridine orange. The image obtained looked like a "comet" with a distinct head comprising of intact DNA and a tail, consisting of damaged or broken pieces of DNA hence the name. The more versatile alkaline method of the comet assay was given by Singh and co workers in 1988. This method was developed to measure DNA damage with high sensitivity.	ENPRA	Institute of Anatomy, Division of Histology, University of Bern	Tue Jan 27 2015
ENMNSC-Protocol-10-1	Development of a Particle Size Sampler for Biological Exposure Studies <small>Published: Yes</small> Download	RESEARCH Owner	In this study, a Selective Particle Size (SPS) sampler was developed, which is able to provide continuous delivery of diesel soot particles of specific size to a SPS sampler, it is possible to obtain two aerosol streams with different size distributions, suitable for biological exposure studies. A cell exposure protocol is described here.			
ENMNSC-Protocol-11-1	Detecting HO-1 and IL8 by q-PCR <small>Published: Yes</small> Download	RESEARCH Owner	The protocol describes the method to detect HO-1 and IL8 by quantitative real-time PCR.			
ENMNSC-Protocol-12-1	Detection and semi-quantification of Endotoxin Contaminations in NanoParticle Suspensions <small>Published: Yes</small> Download	RESEARCH Owner	In vitro endotoxin test for the detection and semi-quantification of endotoxin in aqueous nanoparticle suspensions using Limulus amoebocyte lysate (LAL).			
ENMNSC-Protocol-13-1	Profiling of the nanomaterial-protein corona <small>Published: Yes</small> Download	RESEARCH Owner	Due to their high free surface energy, most likely all nanomaterials adsorb proteins upon contact with any (biological) fluid. In particular, proteins rapidly adsorb to nanoparticles forming a biological coating around the nanoparticle known as the protein corona. Hence, "naked" nanomaterials in general are expected to behave differently in biological environments only for a short time (< 1min). Therefore, the biomolecular corona of nanomaterials need to be considered as novel materials with different properties compared to the pristine nanomaterials during their manufacturing. Particularly, the protein corona interacts with biological systems and thus, constitutes a major element of the nanomaterial identity. As such, the protein corona will also (co) determine the nanotoxicity of the nanomaterial, including ecotoxicology, and may influence success of nanomedicine applications.			

Search:

github.com/enanomapper

Search GitHub Explore Gist Blog Help



eNanoMapper

Funded from the European Union's FP7 for research, technological development and demonstration under grant agreement no 604134.

<http://enanomapper.net/>

Filters Find a repository... [+ New repository](#)

nmdataparser Java ★ 0 0

Parsers for different NM data formats

Updated 19 minutes ago

toxbank-api-server Java ★ 0 3

Forked from ToxBank/toxbank-api-server


ToxBank Protocol service

Updated 5 days ago



Modelling Infrastructure

- Web service standards for modelling:
<http://enanomapper.ntua.gr:8080/jaqpot/swagger/>

 **Jaqpote Quattro** <http://enanomapper.ntua.gr:8880/jaqpot/services/api-d> [AQIC5wM2LY4SfczIqjwPxhwl](#) **Explore**

dataset : Dataset API	Show/Hide	List Operations	Expand Operations	Raw
pmmi : PMML API	Show/Hide	List Operations	Expand Operations	Raw
bibtex : BibTeX API	Show/Hide	List Operations	Expand Operations	Raw
enanomapper : eNM API	Show/Hide	List Operations	Expand Operations	Raw
model : Models API	Show/Hide	List Operations	Expand Operations	Raw
task : Tasks API	Show/Hide	List Operations	Expand Operations	Raw
algorithm : Algorithms API	Show/Hide	List Operations	Expand Operations	Raw
aa : AA API	Show/Hide	List Operations	Expand Operations	Raw
feature : Feature API	Show/Hide	List Operations	Expand Operations	Raw
user : Users API	Show/Hide	List Operations	Expand Operations	Raw

[BASE URL: <http://enanomapper.ntua.gr:8880/jaqpot/services/api-docs>]





Collaborations

NanoSafety
Cluster



- **EU NanoSafety Cluster Working Groups & Meetings:**
 - Active contribution (including leadership) to the working groups: WG4 (Databases, lead by Egon Willighagen), WG5 (Modelling), WG7 (Dissemination & Training) and WG8 (Systems Biology)
- **eNM is part of the Harmonization Initiative**
 - Interacting with project such as NanoPuzzles.
 - Piloting ISA-TAB-Nano in collaboration with the Oxford ISA group.
 - NECID (Nano Exposure and Contextual Information Database)
- **OpenTox**
 - Active participation in workgroups and conferences to advance open tox/risk/safety computing standards.
- **The associate partner program was successfully established and implemented**

OpenTox





Collaborations

... with NanoSafety Cluster Projects



– **MARINA:** Import & harmonization of datasets, data templates, available in data.eNanoMapper.net



– **ModNanoTox:** Data harmonization and import into data.eNanoMapper.net



– **NANO REG & ProSafe:** Ontology input, data harmonization (OECD templates, ISA-TAB-Nano implementation), importing datasets, database development



– **NANOSOLUTIONS:** Data management agreement





Collaborations

... with NanoSafety Cluster Projects



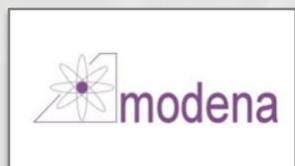
- **SUN & GUIDEnano:** Harmonization initiative for modelling and tools.
- **SUN & RIVM:** Creating a modelling infrastructure, based on PROAST and integrating it into the SUN DSS as federated services.
- **NanoFASE, GUIDEnano, SUN:** Joint training activities in hands-on workshop (10 Feb 2016).





Collaborations

... with NanoSafety Cluster Projects



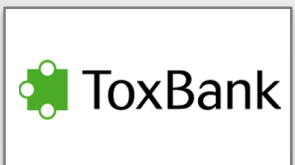
- **COST Action MODENA:** Syracuse meeting contribution, Co-organised CompNanoTox Meeting in Malaga.



- **CEN/CENELEC:** Forming a collaboration agreement, member of workgroup CEN/TC 352



- ... **NanoPuzzles, NanoDefine, FutureNanoNeeds, ToxBank etc.**



eNanoMapper events 2016

Exploitation Seminar

- *Event organized during the 2nd Annual Meeting of eNanoMapper, where all partners will be represented*
- 8-9 February 2016, Basel, Switzerland

Hands-on workshop on Nano Safety Assessment

- *Joint event of eNanoMapper, NanoFASE, GUIDEnano and SUN projects*
- eNM members (DC, UM, IDEA, IST, NTUA and MB) will lead various workshop sessions
- 10 Feb 2016, Basel, Switzerland

2nd eNM ontology workshop/hackathon

- *UM will co-organize this event, together with NECID*
- 3 March 2016, (TNO, Leiden, Netherlands)

2nd Nanosafety Forum for Young Scientists,

- *In conjunction with NanoSafety Cluster Autumn Meeting*
- *Organizer: KI, in collaboration with the WGs in the Cluster*
- Mid-September 2016, Visby, Gotland, Sweden

Final eNM Conference

- exact date and location to be decided



HANDS-ON WORKSHOP ON NANO SAFETY ASSESSMENT

10 February 2016, Technology Park, Basel

- This joint event is bringing together inputs and approaches from several EU NMP projects (e.g. eNanoMapper, NanoFASE, GUIDEnano, SUN)



Objectives

- To work through nanotechnology safety examples and exercises using existing data resources and modelling tools;
- To use information in support of nanotechnology risk assessment goals and to discuss current results;
- To discuss the role of harmonisation and ontology in the use of multiple modelling and assessment tools applied to nano safety.



Format

- The workshop will focus on specific cases and practical examples in which the group will work through modelling, analysis and assessment exercises, and discuss the results.

<http://www.enanomapper.net/events/workshop-basel-2016>



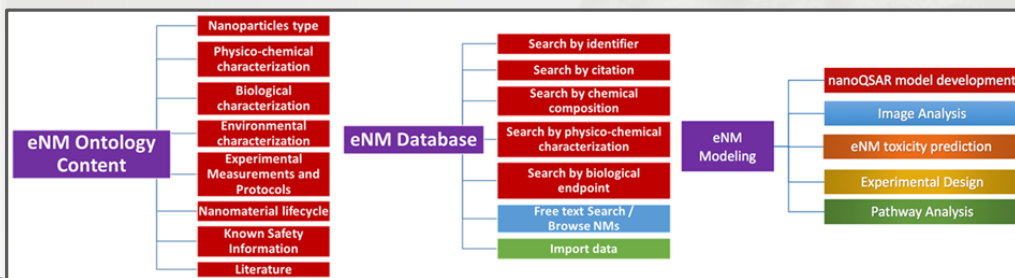


Application Map: The Portal to the eNanoMapper Applications

Portal for all eNanoMapper applications.

- A quick, simple and easy entry point for anyone to all applications developed by the project.

<http://eNanoMapper.net/applications>





NanoEHS Communities of Research and the 'Taj Mahal' Project

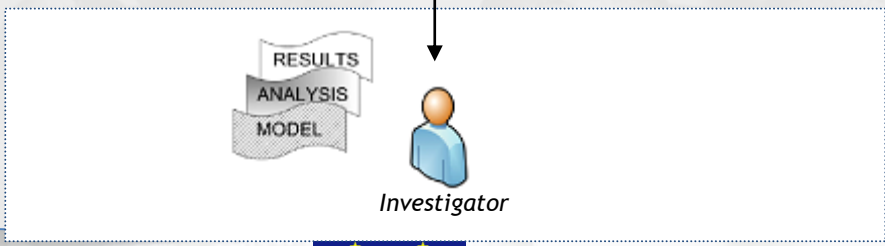
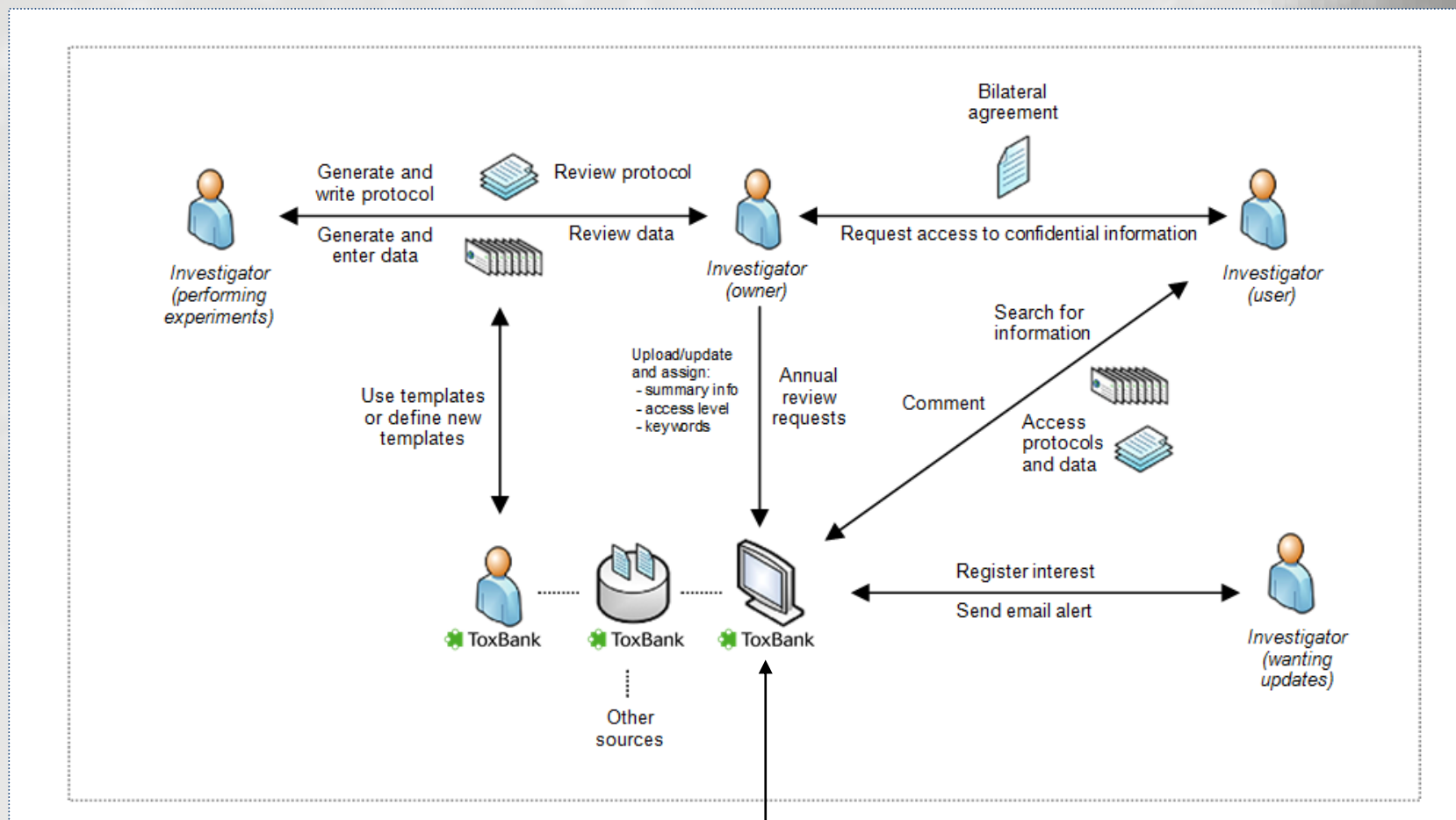
- Leadership of CoR on Databases & Computational Modelling.
- Leading the case study supporting applications for the scrimmage.
 - Supporting the capturing of the solution.
 - Guiding and pre-structuring the solution process and resources.
 - Providing and co-developing a framework of applications and resources

Apply to Decision Making, Guidance Development, White papers, Crisis Situations

us - eu
bridging nanoEHS research efforts



Data Sharing within ToxBank



Sustainability

- **Develop Data & Modelling Science Community**
- **Develop Community infrastructure activities aligned with NS Cluster**
- **Community & Network Funding – e.g., Infrastructure, COST, Marie Curie**
- **Join/align with open commercial approaches e.g., OpenTox, ToxBank – non profit organisation with open standards and business ecosystem**
- **Establishment of acceptance and international use of Ontology**
- **Interactions with the Publishing industry (Open Access Models)**
- **Medium term public funding - Infrastructure proposal?**
- **Operationalise Business Ecosystem Model, Services and Support**



Project Consortium

Douglas Connect
Working communities




in silico toxicology

IOFA
consult



**Karolinska
Institutet**



EMBL-EBI 



Maastricht University

misvik biology 

