eNanoMapper - a Database and Ontology Framework for Design and Safety Assessment of Nanomaterials

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Nanoparticles type

Physico-chemical

characterization

Environmental

Experimental

Measurements and

Protocols

lanomaterial lifecycle

Known Safety

http://www.nanosafetycluster.eu/



http://enanomapper.net

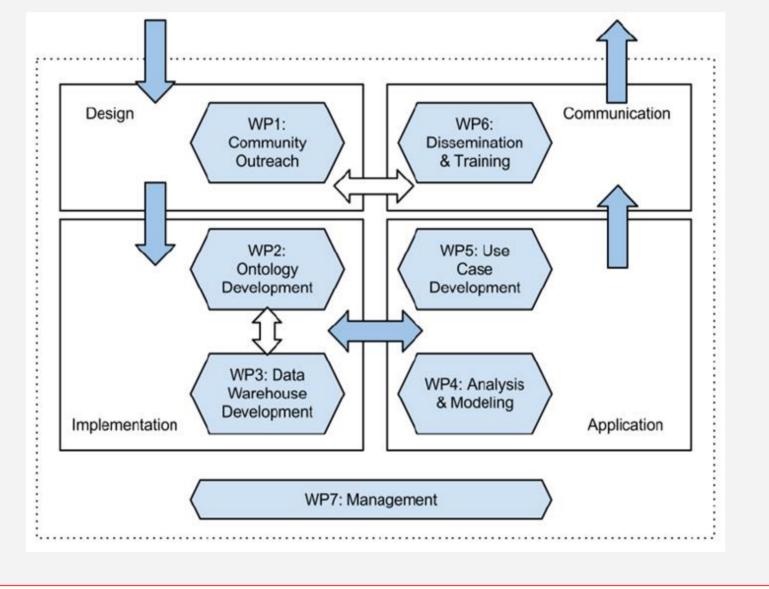
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Main Objectives of eNanoMapper FP7 Project

- 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.

Not to generate a large collection of data, but rather a collection of standards and tools to support the basis of a "smart" database with a wide variety of functions and application areas.

Structure and Work-flow



The eNanoMapper Ontology

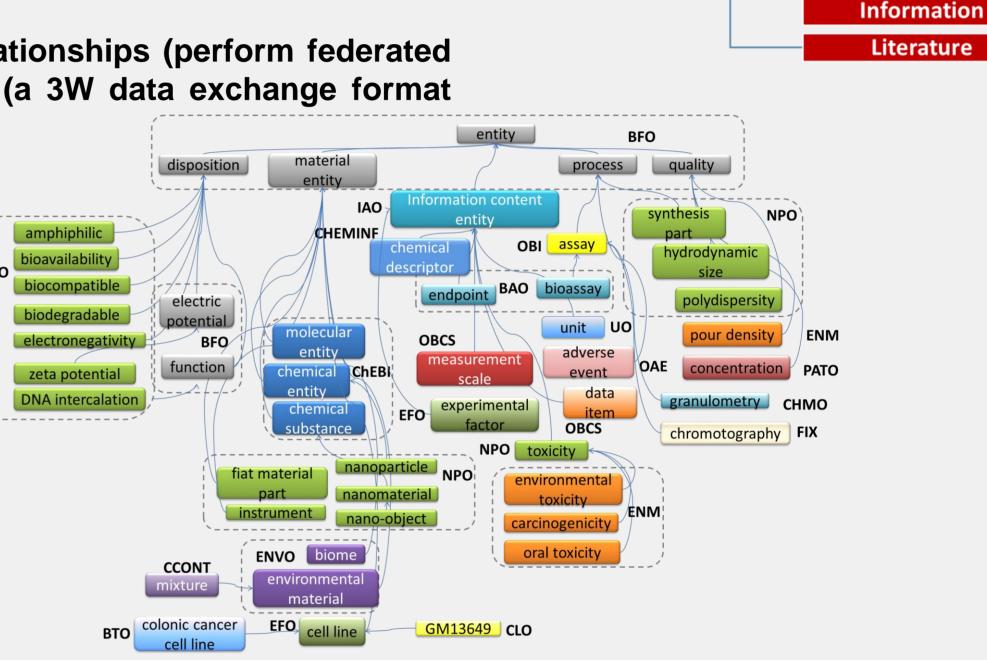
An ontology is a controlled vocabulary built on the relationships hierarchical between metaphysical term concerned with the nature and relations of being.

Principal questions include:

What can be said to exist? What is a thing? Into what categories, if any, can we sort existing things? What are the meanings of being? What are the various modes of being of entities?

<u>Usage:</u>

- Harmonize data from several sources to one database.
- To analyze for relationships (perform federated SPARQL queries) (a 3W data exchange format is used).

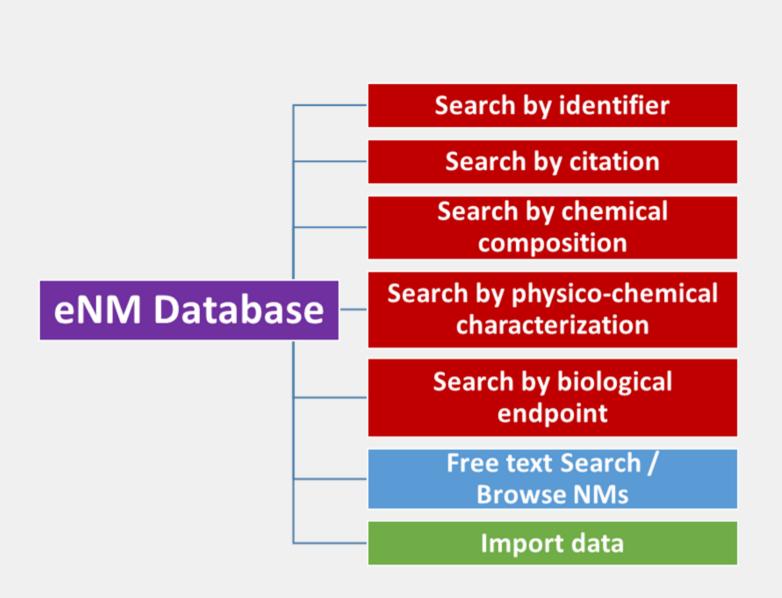


eNM Ontology

Content

The eNM Ontology assembled from multiple sources (1)

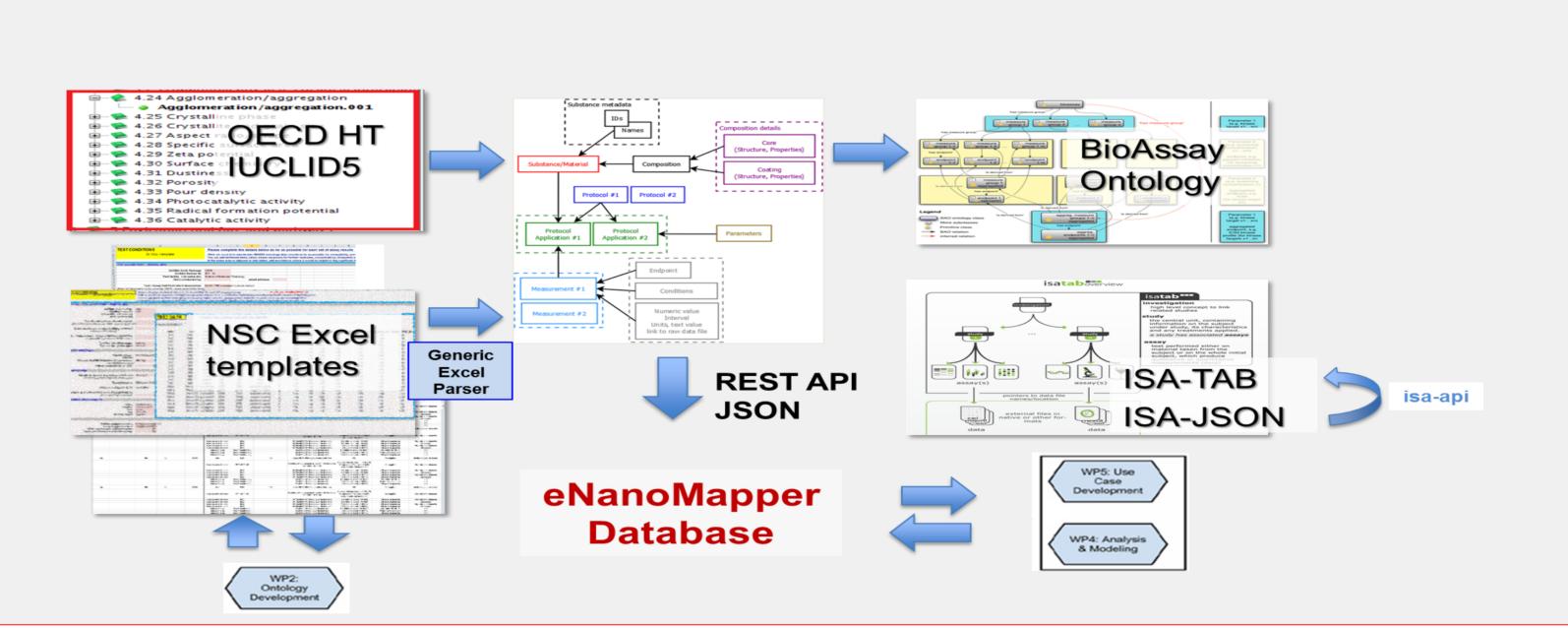
The eNanoMapper Database



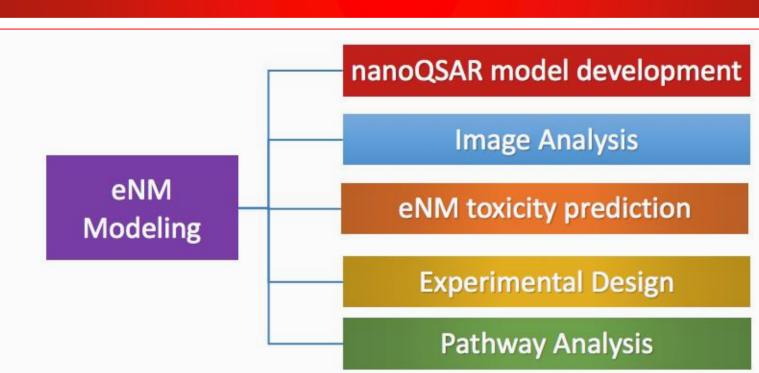
- Based on OpenTox API
- Open Source implementations
- Multiple data exchange format
- ISA-TAB (and ISA-JSON), semantic formats,
 - OECD HT
- formats for machine learning packages, etc.
- Bridging with data analysis tools (conjoiner service)
- Linking to other major data collection/databases (2)

Implementation of a database structure with the necessary provisions for data protection, data sharing, data quality assurance, searchability, tailored interfaces for different needs and usages, comparability and cross-talk with other databases.

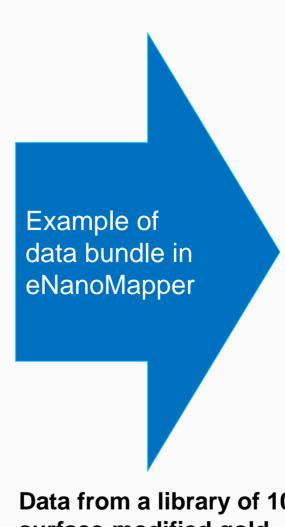
https://data.enanomapper.net/



eNanoMapper Modelling Tools



- A user-friendly interface that enables access to eNanoMapper Jaqpot Quattro tools and applications, but also to a repository of validated models (http://www.jaqpot.org)
- RRegrs R package is a collection of R regression tools aiming to find optimal and well validated QSAR models with applications to chemoinformatics and nanotoxicology data(3)
- The conjoiner service links the eNM database with the modelling platform. It transforms experimental data into a modelling-friendly format, and produces standardized datasets.
- Raw data of nanomaterials such as images, crystallographic data and proteomics data, are processed by descriptor calculation services to produce compact and informative numerical descriptors.
- Data modelling and analysis services implement computational experimental design methods, tools for interlaboratory proficiency testing and non-testing approaches for predicting toxicity and for filling data gaps (NanoQSAR and read-across methods).
- A number of mechanistic modelling tools combine experimental data with information from public biological databases and tools to perform pathway and network analysis.



Data from a library of 105 surface-modified gold nanoparticles

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□ - 12 - ■	G15.DDT@CTAB	FCSV-d1731b11-2	nanoparticle		G15.DDT@CTAB		FCSV-d1731b11-2		Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv			Classificat
□ - 13 - □	G15.DDT@DOTAP	FCSV-3b96ad7a-b	ad7a-b nanoparticle		G15.DDT@DOTAP		FCSV-3b96ad7a-b		Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv			Classificat
□ - 14 - ►	G15.DDT@ODA	FCSV-fb5e6048-8	nanoparticle		G15.DDT@ODA		FCSV-fb5e6048-8 Protein C		Protein Cor	orona Fingerprinting Predicts ar Interaction of Gold and Silver		Classificat
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□ - 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			Classificat
□ - 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			Classificat
□ - 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			Classificat
	30.DDT@CTAB <u>FCSV-c4e9df58-f</u> nanoparticle		G30.DDT@CTAB		€ the		Protein Cor	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv				

- 1) Hastings et al. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics. December 2015, 6:10
- 2) Jeliazkova et al. The eNanoMapper database for nanomaterial safety information. Beilstein Journal of Nanotechnolgy 2015, 6, 1609-1634
- Tsiliki et al. RRegrs: an R package for computer-aided model selection with multiple regression models. Journal of Cheminformatics 2015, 7:46

http://enanomapper.net

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