

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

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<http://enanomapper.net>

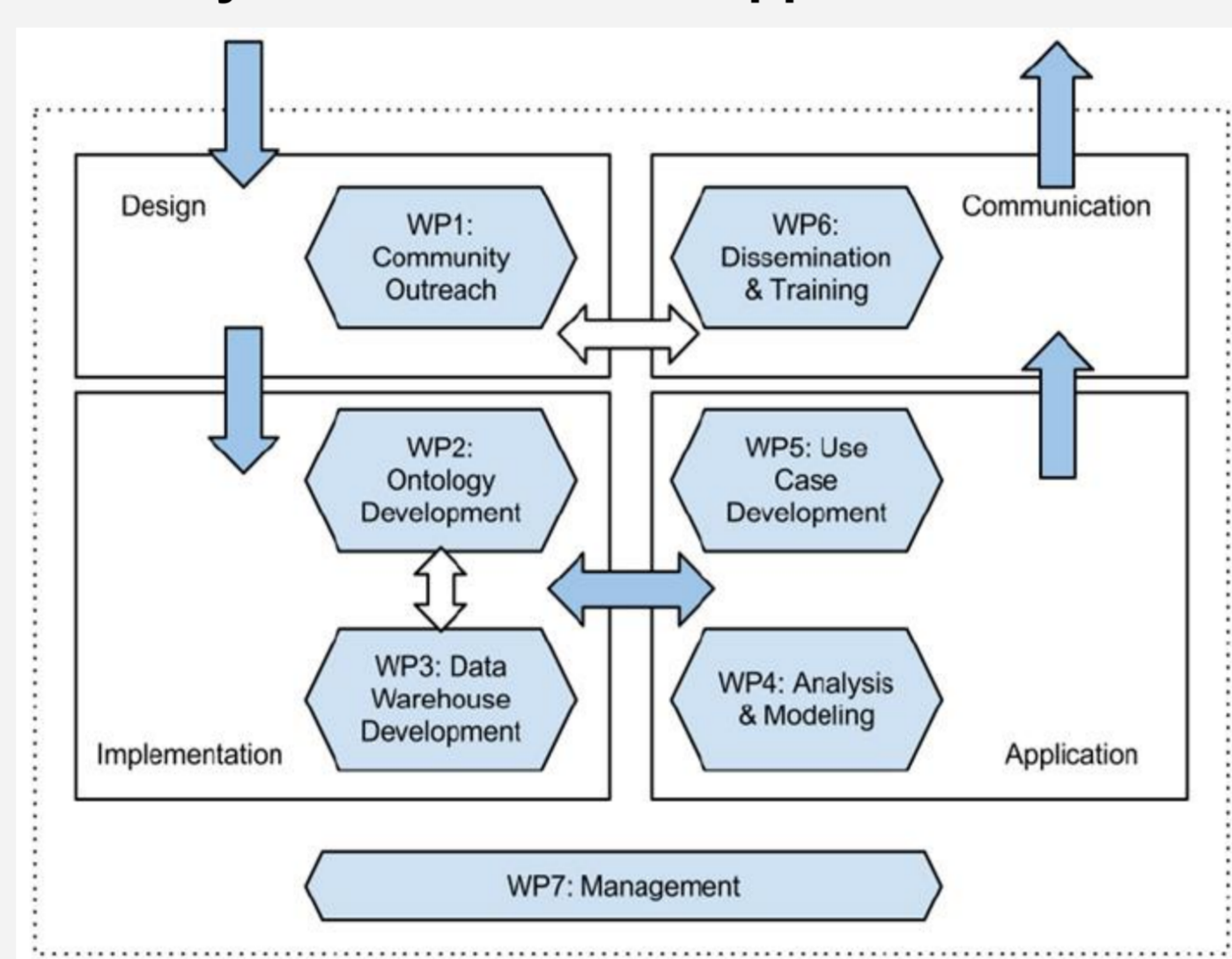
<http://www.nanosafetycluster.eu>

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

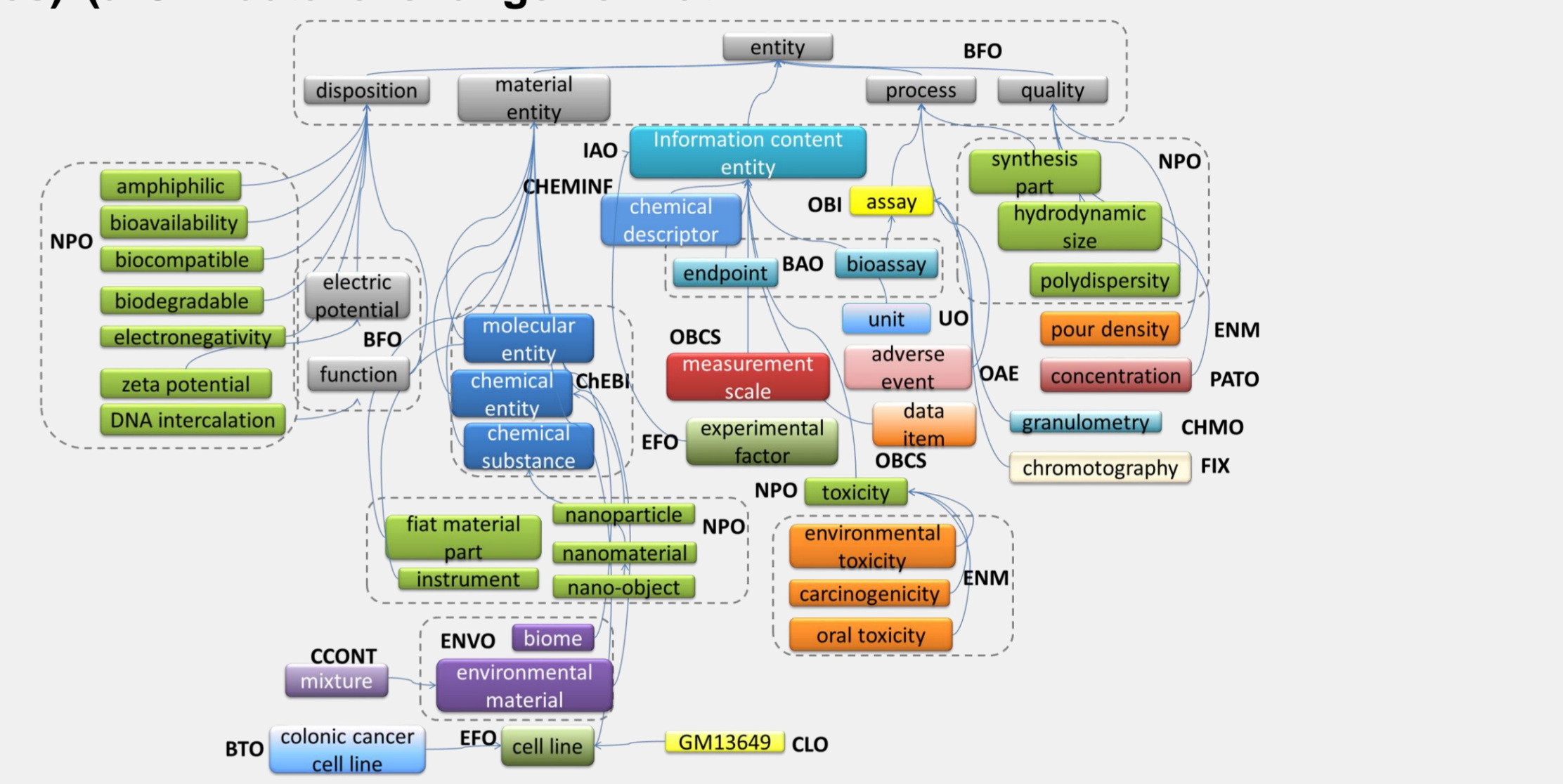
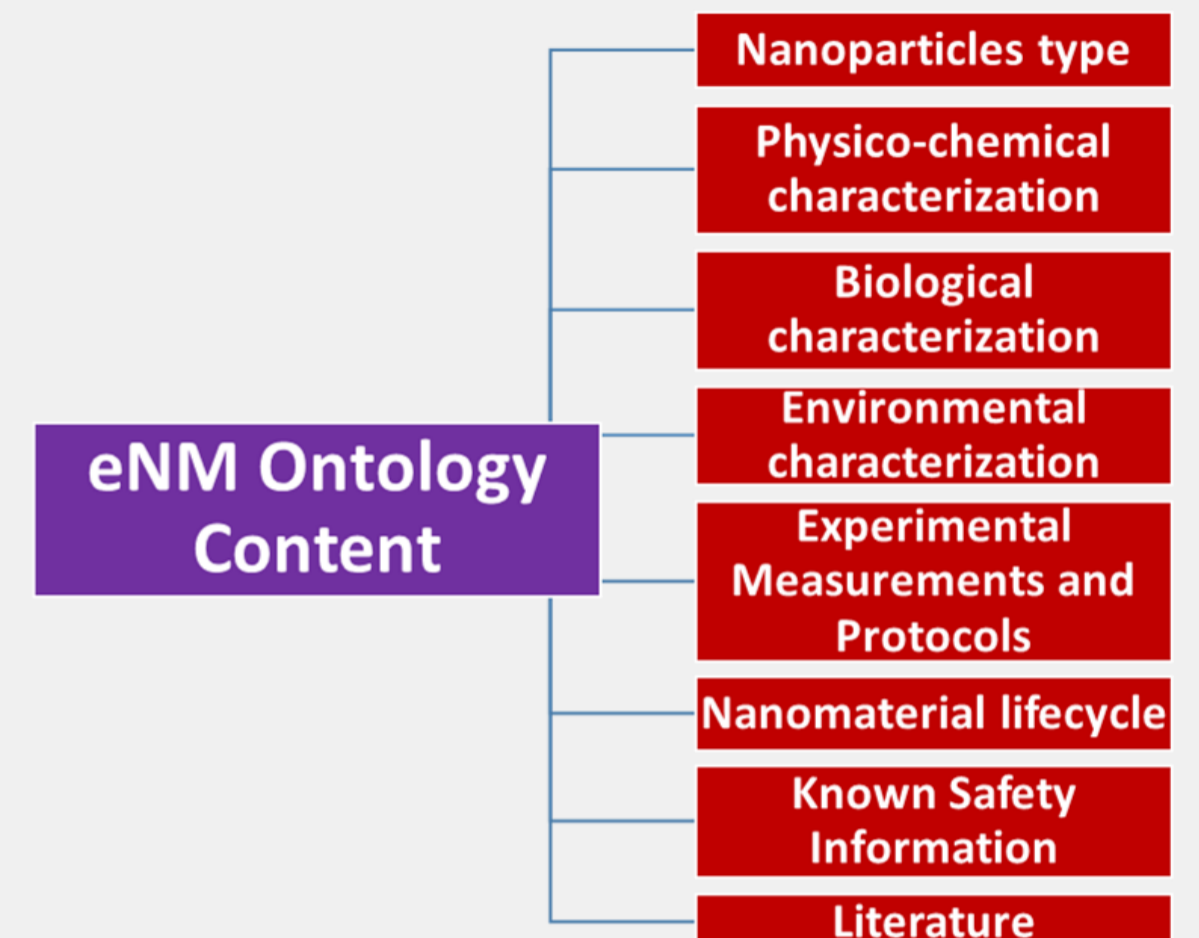
An ontology is a controlled vocabulary built on the hierarchical relationships between terms; a metaphysical term concerned with the nature and relations of being.

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?

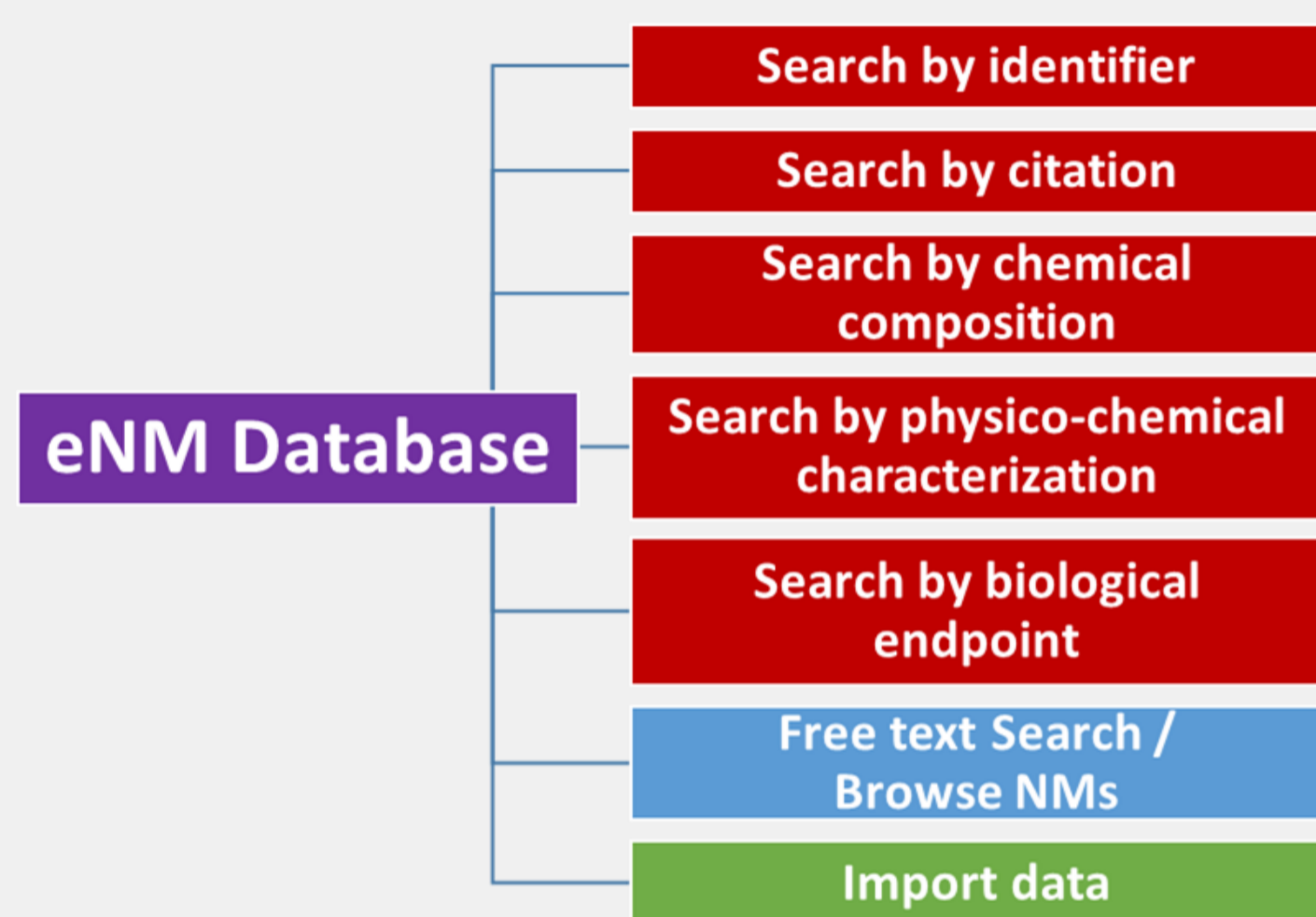
Usage:

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



The eNM Ontology assembled from multiple sources (1)

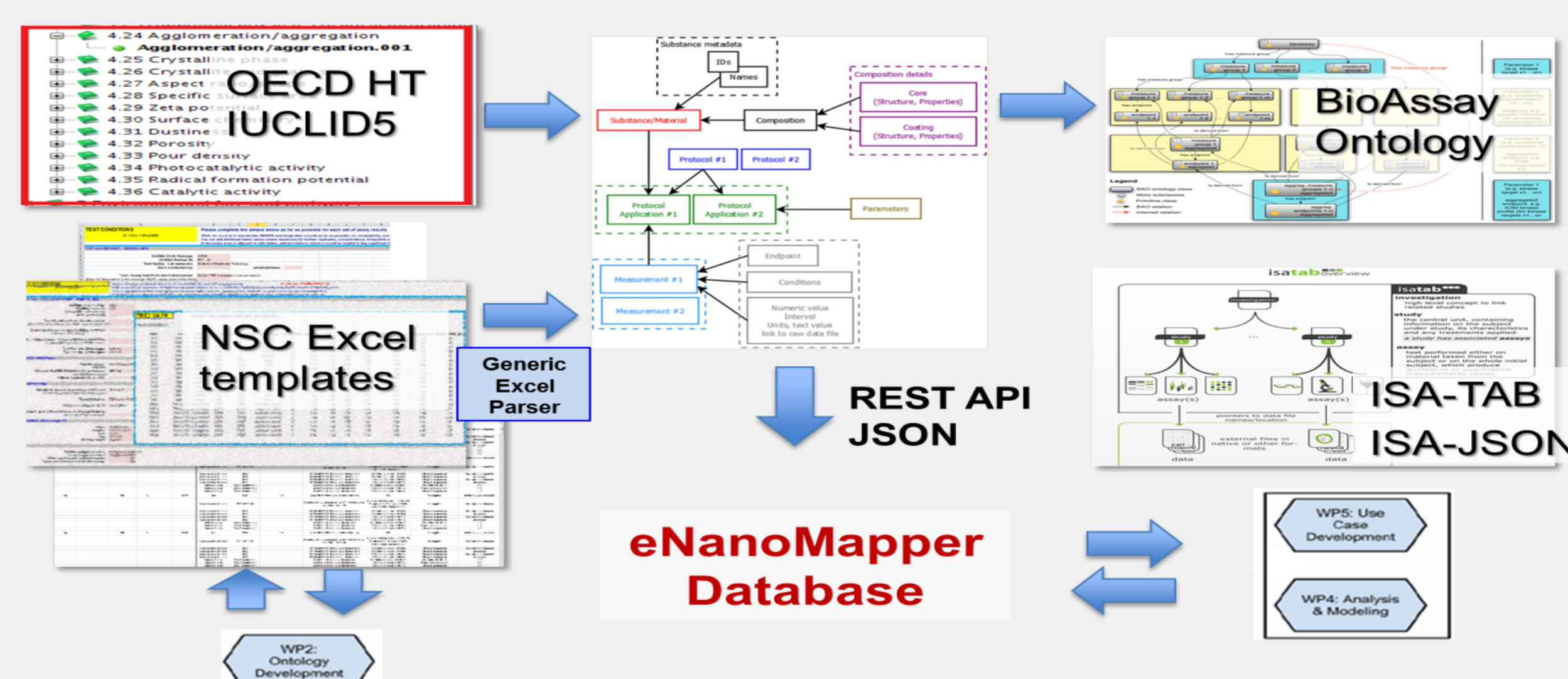
The eNanoMapper Database



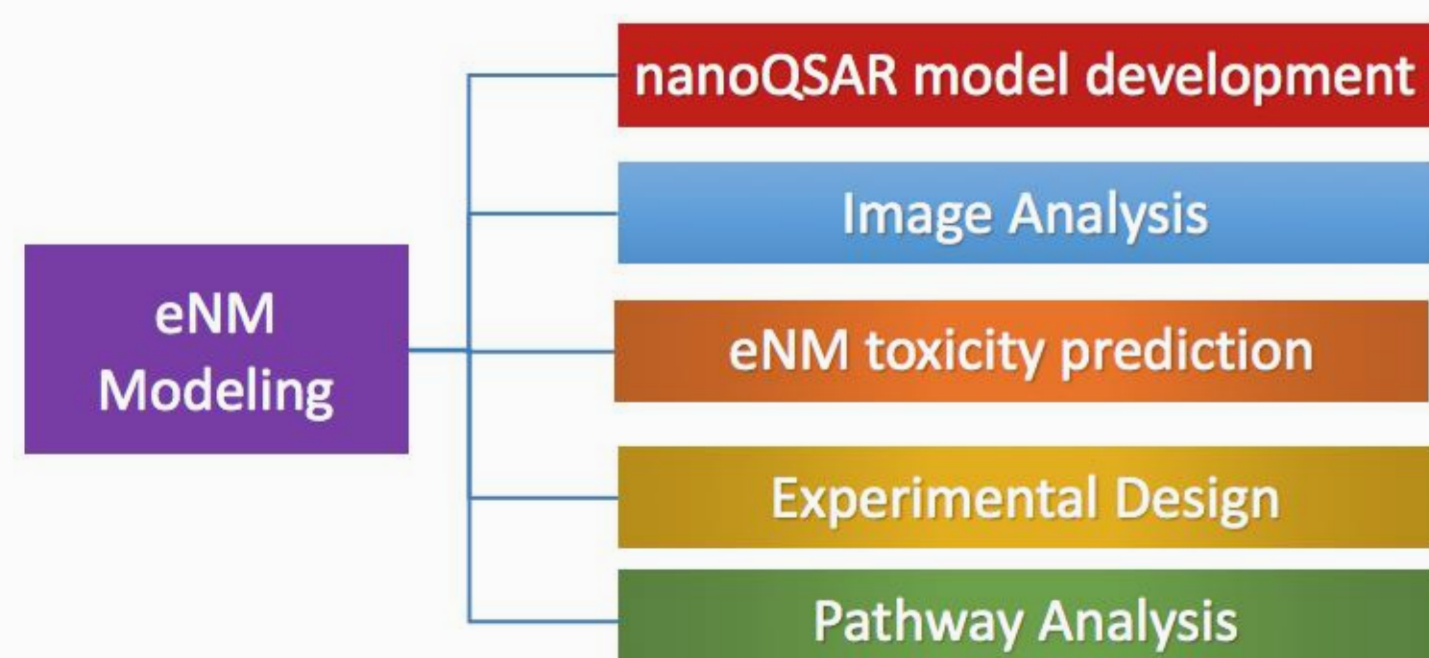
- Based on OpenTox API
- Open Source implementations
- Multiple data exchange format
 - ISA-TAB (and ISA-JSON), semantic formats,
 - OECD HT
 - formats for machine learning packages, etc.
- Bridging with data analysis tools (conjoiner service)
- Linking to other major data collection/databases (2)

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 cheminformatics 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**.

Example of data bundle in eNanoMapper

Data from a library of 105 surface-modified gold nanoparticles

1) Hastings et al. **eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment.** Journal of Biomedical Semantics. December 2015, 6:10

2) Jeliaskova et al. **The eNanoMapper database for nanomaterial safety information.** Beilstein Journal of Nanotechnology 2015, 6, 1609–1634

3) 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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