

Abstract

During the eNanoMapper project *in silico* toxicologies (IST) public services were adapted to the specification of the eNanoMapper API and new nanoparticle specific developments were implemented. This poster depicts the interaction of IST services with eNanoMapper resources of other partners which covers use cases like data download/mirroring, augmentation of GUIs with ontology queries and nanoparticle descriptor calculation.

Links

- ▶ eNM data warehouse <https://data.enanomapper.net>
- ▶ eNM ontologies <https://github.com/enanomapper/ontologies>
- ▶ nano-lazar GUI <https://nano-lazar.in-silico.ch>
- ▶ eNM ontology viewer <https://query.enanomapper.net/enm-viewer>
- ▶ nano-lazar REST interface <https://enm.in-silico.ch>
- ▶ eNM SPARQL interface <https://sparql.enanomapper.net>
- ▶ BioPortal <http://bioportal.bioontology.org>
- ▶ UniProt <http://www.uniprot.org/uniprot>

References

[1] Christoph Helma, Micha Rautenberg, and Denis Gebele. nano-lazar: Read across predictions for nanoparticle toxicities with calculated and measured properties address. *Frontiers in Pharmacology*, 2017. Submitted to Frontiers in Pharmacology 2017 Jan, Predictive Toxicology section.

[2] Christoph Helma, Denis Gebele, and Micha Rautenberg. lazard, December 2016. URL <https://doi.org/10.5281/zenodo.215483>.

[3] Denis Gebele, Micha Rautenberg, and Christoph Helma. nano-lazar, January 2017. URL <https://doi.org/10.5281/zenodo.250818>.

[4] Micha Rautenberg, Denis Gebele, and Christoph Helma. lazard-rest, October 2016. URL <https://doi.org/10.5281/zenodo.187328>. source code for this version on Github: <https://github.com/opentox/lazar-rest/tree/v1.0.0>.

Integration details

lazar [1][2]

- ▶ Mirrors eNanoMapper data for read-across models
- ▶ Creates read-across predictions for the nano-lazar webinterface
- ▶ Responds to requests from the lazard-rest interface (e.g. nanoparticle predictions, model creation and validation, descriptor calculation)

RDF store

- ▶ Mirrors eNanoMapper data and ontologies
- ▶ Responds to SPARQL queries from the ontology viewer and the SPARQL interface

nano-lazar GUI [3]

- ▶ Obtains nanoparticle toxicity predictions from the lazard library
- ▶ Uses ontologies (eNanoMapper, BioPortal, UniProt) to explain domain specific terms in the user interface
- ▶ Uses ontologies and eNanoMapper data as supporting information for read-across predictions

eNM ontology viewer

- ▶ Sends SPARQL queries to the RDF store
- ▶ Visualises RDF response from the RDF store

nano-lazar REST interface [4]

- ▶ Interacts with the lazard library (e.g. for toxicity predictions, model creation and validation, descriptor calculation)
- ▶ Will be maintained and developed in the FP7 OpenRiskNet project

eNM SPARQL interface

- ▶ Sends SPARQL queries to the RDF store
- ▶ Receives SPARQL query results in different formats

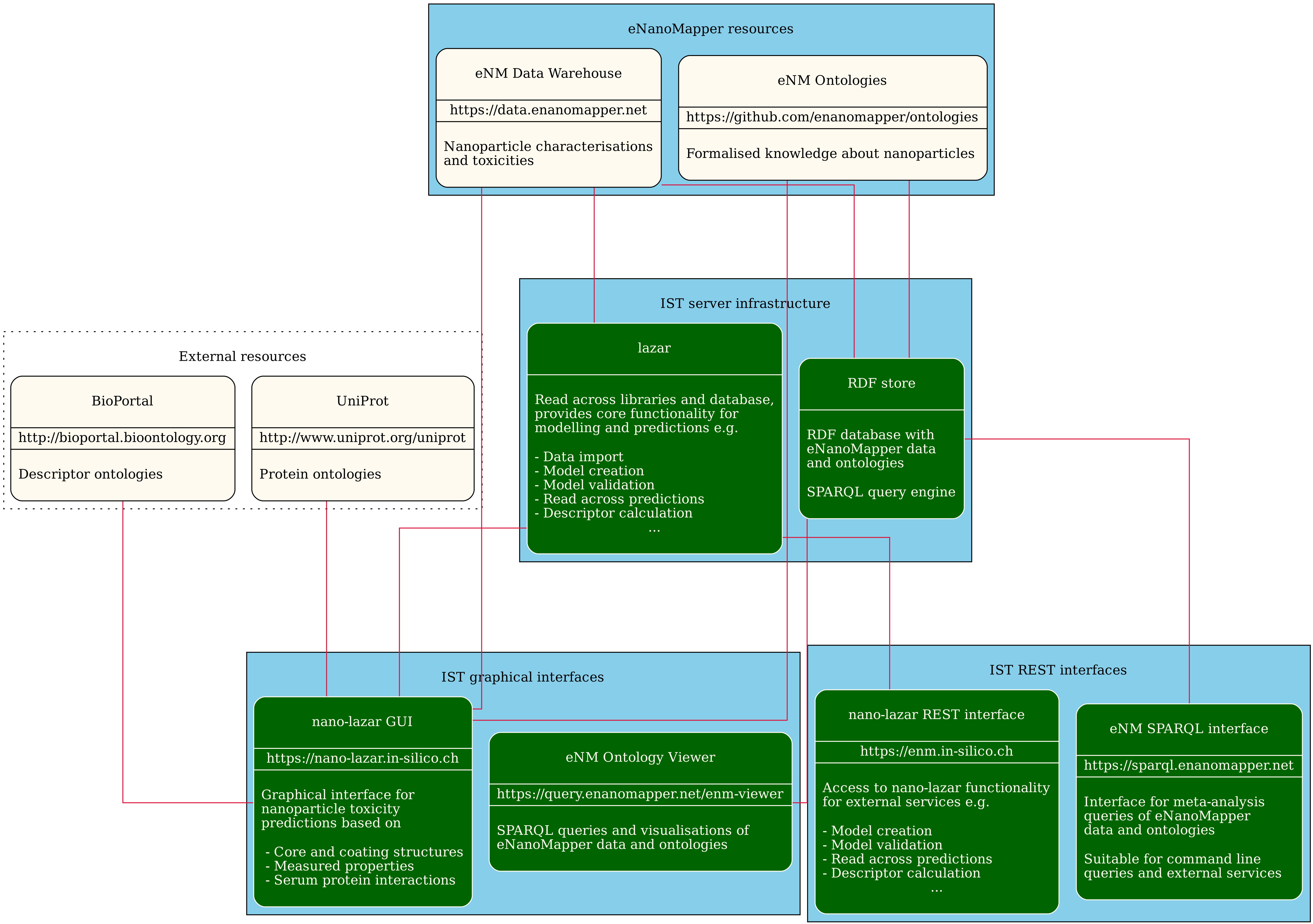


Figure 1: nano-lazar integration