

Abstract

During the eNanoMapper project *in silico* toxicologies (IST) public server infrastructure was adapted to the requirements of the eNanoMapper project and augmented with new developments. This poster gives a comprehensive overview of all IST resources developed within eNanoMapper. Each service is presented with a brief description and links to the public interface, source code, documentation and download links for self-contained docker images.

lazar

lazar[1] is a framework for read-across predictions. Within eNanoMapper lazarus was extended with interfaces for the eNanoMapper infrastructure and capabilities to predict nanomaterial toxicities.

- ▶ lazarus source code [2] <https://github.com/opentox/lazar>
- ▶ lazarus Ruby gem library <https://rubygems.org/gems/lazar>
- ▶ lazarus issue tracker <https://github.com/opentox/lazar/issues>
- ▶ lazarus methodology and validation <https://github.com/enanomapper/nano-lazar-paper/blob/master/nano-lazar.pdf>
- ▶ lazarus tutorial <https://github.com/opentox/lazar/blob/master/README.md>
- ▶ lazarus API documentation <http://www.rubydoc.info/gems/lazar>

nano-lazar

The nano-lazar GUI provides a public webinterface for nano-lazar models.

- ▶ nano-lazar public webinterface [3] <https://nano-lazar.in-silico.ch>
- ▶ nano-lazar source code <https://github.com/eNanoMapper/nano-lazar>
- ▶ nano-lazar Ruby gem library <https://rubygems.org/gems/nano-lazar>
- ▶ nano-lazar issue tracker <https://github.com/eNanoMapper/nano-lazar/issues>
- ▶ nano-lazar API documentation <http://www.rubydoc.info/gems/nano-lazar>
- ▶ nano-lazar dockerized service on Docker Hub <https://hub.docker.com/u/insilicotox/nano-lazar>

nano-lazar-paper

Detailed description of nano-lazar methods and validation results [4]. Results can be reproduced by external researchers with the accompanying docker image.

- ▶ Source code for nano-lazar publication (and oral presentations). <https://github.com/enanomapper/nano-lazar-paper>
- ▶ Manuscript submitted to Frontiers in Pharmacology <https://github.com/enanomapper/nano-lazar-paper/blob/master/nano-lazar.pdf>
- ▶ Tutorial for repeating nano-lazar validation experiments <https://github.com/enanomapper/nano-lazar-paper/blob/master/README.md>
- ▶ Docker image for inspection and reproduction of validation experiments <https://hub.docker.com/r/insilicotox/nano-lazar-paper/>

lazar-rest

lazar-rest provides an eNanoMapper compatible REST API for the nano-lazar read-across framework.

- ▶ lazarus-rest Swagger UI documentation for API visualization and interaction [5] <https://enm.in-silico.ch>
- ▶ lazarus-rest Swagger API definition file <https://enm.in-silico.ch/api/api.json>
- ▶ lazarus-rest source code <https://github.com/opentox/lazar-rest>
- ▶ lazarus-rest Ruby gem library <https://rubygems.org/gems/lazar-rest>
- ▶ lazarus-rest issue tracker <https://github.com/opentox/lazar-rest/issues>
- ▶ lazarus-rest API documentation <http://www.rubydoc.info/gems/lazar-rest>

SPARQL endpoint to eNM ontology and data

SPARQL query interface for eNanoMapper data and ontologies

- ▶ SPARQL endpoint <https://sparql.enanomapper.net/>
- ▶ Documentation http://enanomapper.net/deliverables/d3/20160420_eNanoMapper_D3.2_Data_Management_System_with_extended_search_capabilities_FINAL.pdf

eNM ontoviewer

The eNanoMapper ontology viewer visualizes SPARQL query results from eNM ontologies and data.

- ▶ eNanoMapper ontology viewer [6] <https://query.enanomapper.net/>
- ▶ eNanoMapper ontology viewer source code <https://github.com/enanomapper/enm-ontoviewer>
- ▶ eNanoMapper ontology viewer issue tracker <https://github.com/enanomapper/enm-ontoviewer/issues>

QSAR-reporting

QMRF and QPRF reporting features for nano-lazar. This library is accessible from the nano-lazar GUI and the lazarus-rest webservice.

- ▶ qsar-report source code [7] <https://github.com/opentox/qsar-report>
- ▶ qsar-report Ruby gem library <https://rubygems.org/gems/qsar-report/>
- ▶ qsar-report issue tracker <https://github.com/opentox/qsar-report/issues>
- ▶ qsar-report tutorial <http://opentox.github.io/usage/2016/10/05/qmrf-and-qprf-reporting-library-gem>
- ▶ qsar-report API documentation <http://www.rubydoc.info/gems/qsar-report>

Authorization & Authentication

Infrastructure for eNanoMapper authentication and authorization.

- ▶ Single sign-on authorization & authentication service <https://openam.in-silico.ch/openam/>

eNanoMapper infrastructure

eNanoMapper infrastructure services implemented and maintained by IST.

- ▶ Bugzilla issue tracker for eNanoMapper <https://bugzilla.enanomapper.net/>
- ▶ Mailman mailing list for partner, developers and associate-partners <http://lists.enanomapper.net/cgi-bin/mailman/listinfo/partner> <http://lists.enanomapper.net/cgi-bin/mailman/listinfo/developers> <http://lists.enanomapper.net/cgi-bin/mailman/listinfo/associate-partner>
- ▶ Registration form and user management <https://purl.enanomapper.net/register/>
- ▶ Online visualization of eNanoMapper specification documents <http://specs.enanomapper.net>
- ▶ Maintenance for scripts to query the eNM ontology at purl.enanomapper.net (e.g. https://purl.enanomapper.net/php/ENM_0000018)
- ▶ LDAP user database server and replication server <http://ldap.opentox.org>
- ▶ Blog entries with technical details about eNanoMapper implementations <http://opentox.github.io/archive>

Testing framework

IST uses the Ruby MiniTest framework for Test Driven Development (TDD). Automated nightly tests keep track of code changes and ensure the interoperability within IST components and with external services.

References

- [1] Andreas Maunz, Martin Gütlein, Micha Rautenberg, David Vorgrimmmler, Denis Gebele, and Christoph Helma. lazarus: a modular predictive toxicology framework. *Frontiers in Pharmacology*, 4, 2013. doi: 10.3389/fphar.2013.00038. URL <http://dx.doi.org/10.3389/fphar.2013.00038>.
- [2] Christoph Helma, Denis Gebele, and Micha Rautenberg. lazarus, 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] 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.
- [5] Micha Rautenberg, Denis Gebele, and Christoph Helma. lazarus-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>.
- [6] Denis Gebele, Micha Rautenberg, and Christoph Helma. eNanoMapper ontology viewer, January 2017. URL <https://doi.org/10.5281/zenodo.259384>.
- [7] Micha Rautenberg, Christoph Helma, and Denis Gebele. qsar-report Ruby gem library, September 2016. URL <https://doi.org/10.5281/zenodo.179038>.