In silico toxicology services for nanoparticle risk assessment

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

- lazar source code [1] https://github.com/opentox/lazar
- lazar Ruby gem library https://rubygems.org/gems/lazar
- lazar issue tracker https://github.com/opentox/lazar/issues
- lazar methodology and validation https://github.com/enanomapper/nano-lazar-paper/blob/master/nano-lazar.pdf
- lazar tutorial https://github.com/opentox/lazar/blob/master/README.md
- lazar 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 [2] 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 [3]. 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.

- lazar-rest Swagger UI documentation for API visualization and interaction [4] https://enm.in-silico.ch
- lazar-rest Swagger API definition file https://enm.in-silico.ch/api/api.json
- lazar-rest source code https://github.com/opentox/lazar-rest
- lazar-rest Ruby gem library https://rubygems.org/gems/lazar-rest
- lazar-rest issue tracker https://github.com/opentox/lazar-rest/issues
- lazar-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 [5] 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 lazar-rest webservices.

- qsar-report source code[6] 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] Christoph Helma, Denis Gebele, and Micha Rautenberg. lazar, December 2016. URL https://doi.org/10.5281/zenodo.215483.

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

[3] 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.

[4] Micha Rautenberg, Denis Gebele, and Christoph Helma. lazar-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.

[5] Denis Gebele, Micha Rautenberg, and Christoph Helma. eNanoMapper ontology viewer, January 2017. URL https://doi.org/10.5281/zenodo.259384.

[6] Micha Rautenberg, Christoph Helma, and Denis Gebele. qsar-report Ruby gem library, September 2016. URL https://doi.org/10.5281/zenodo.179038.

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