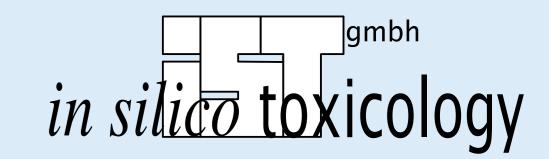


In silico toxicology eNanoMapper REST services

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Abstract

During the eNanoMapper project *in silico* toxicologies (IST) webservices were adapted in order to provide REST interfaces that adhere to eNanoMapper standards and specifications and supplemented with interactive SWAGGER documentation. This poster gives an overview of ISTs eNanoMapper API compatible REST services[1] and demonstrate its usage with practical examples.

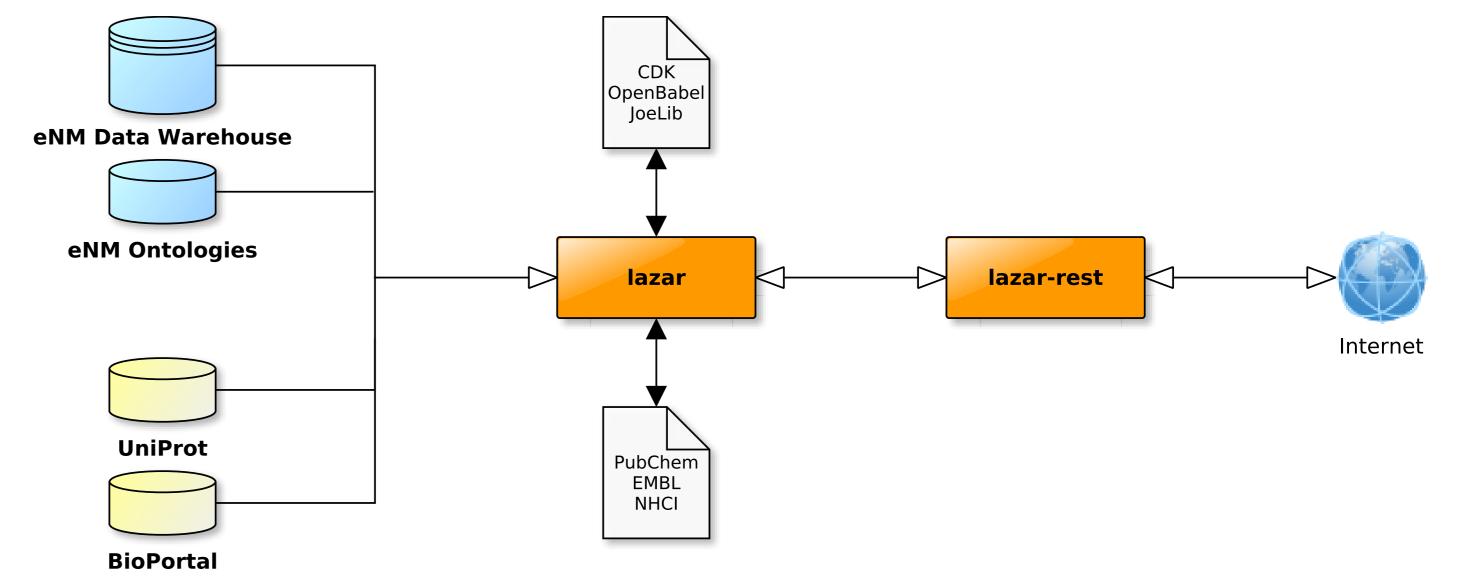
lazar

REST

lazar (lazy structure-activity relationships)[2] is a modular framework for read across predictions of chemical toxicities. Within the European Union's FP7 eNanoMapper project lazar was extended with capabilities to handle nanomaterial data and interfaces to other eNanoMapper services (databases and ontologies). lazar libraries are publicly distributed as Ruby gems.

Integration with eNanoMapper and other services

lazar-rest provides a REST webservice for the nano-lazar framework. The lazar framework integrates internal libraries, eNanoMapper resources (Data Warehouse and Ontologies) and external resources like UniProt and BioPortal. lazar-rest services make the lazar framework accessible for other webservices and web applications and for users who prefer the command line over graphical user interfaces.



Representational State Transfer or RESTful API is an architectural style to design webservices. REST uses HTTP protocol requests GET, POST, PUT, DELETE for the communication between distributed webservices. nano-lazar[3] as a part of the eNanoMapper analysis and modelling infrastructure is built upon the OpenTox web services framework following the principles of the Representational State Transfer (REST) design model.

lazar-rest services

lazar-rest is a Ruby library, that provides a REST interface for nano-lazar. The API is compatible with eNanoMapper specifications and documented with the Swagger API framework (version 2.0), which conforms with the Open API Initiative specification.

lazar-rest Swagger interface

Swagger UI is used as an interactive documentation and visualization platform for the lazar-rest API.



Lazar & Nano-Lazar REST Service

REST API webservice for lazar and nano-lazar. lazar (lazy structure-activity relationships) is a modular framework for predictive toxicology. With activated Authentication & Authorization, subjectid authorization token are obligatory for designated services.

See also *lazar-rest* documentation on Github

https://github.com/opentox/lazar-rest Created by in silico toxicology gmbh See more at <u>www.in-silico.ch</u> <u>Contact the developer</u> <u>GNU GENERAL PUBLIC LICENSE</u> Figure 2: nano-lazar service integration

Authorization & authentication

Data confidentiality, authentication and authorization (AA) is a common requirement for many resources. Within the OpenTox[5] project, *in-silico* toxicology gmbh has implemented a single-sign-on method with an OpenLDAP backend for user management and OpenAM for authentication and authorization. This system was updated and revised for eNanoMapper and provides access control for the current services. Conforming to the OpenTox web service architecture principles[5], eNanoMapper services can be decoupled from AA. This provides the opportunity to deploy a service without AA, if required (e.g. for local installations).

Practical linux cURL command examples

Get an URI list for all models:

curl -X GET --header 'Accept: text/uri-list' -H 'accept:text/uri-list' 'https://enm.in-silico.ch/model'

Retrieve an JSON representation of a model:

curl -X GET -H 'Accept: application/json' -H 'accept: application/json' 'https://enm.in-silico.ch/model/<MODELID>'

Predict a nano-particle:

curl -X POST -H 'Content-Type: application/x-www-form-urlencoded' -H 'Accept:text/html' -d 'identifier= https://enm.in-silico.ch/nanoparticle/<NANOPARTICLEID>' 'https://enm.in-silico.ch/model/<MODELID>'

api : Swagger API representation	in JSON	Show	w/Hide List Operations Expand Oper	rations			
authentication : minimal Authent	tication service	Shov	w/Hide List Operations Expand Oper	rations			
descriptor : Descriptor api	: Swagger API re	presentatio	n in JSON	Show/	Hide List Operations Exp	and Operations	
feature : Feature authentication : minimal			ntication service	Show/	Hide List Operations Exp	and Operations	
model : Lazar Model Service					Get token		
dataset : Dataset				Destroy token			
validation : Validation desc	or			Hide List Operations Exp	and Operations		
report : QMRF Reporting	or						
compound : Compound	or			Descrij			
substance : Substance	/compound/descript	GET /mode	el/{id}				
nanoparticle : Nanoparticle	ure : Feature	Implementat	ion Notes				
mod	lel : Lazar Model	Get model rep					
[BASE URL: / , API VERSION: 1.0.0]	/model	Parameters					
Response Body GET	/model/{id}	Parameter	Value		Description	Parameter Type	Data Type
{ POST	/model/{id}	accept	application/json ~		requested Content-Type	header	string
<pre>"URI": "https://enm.in-silico.cn/model/582093e5ca7837 "_id": { "\$oid": "582b93e5ca78370057b50d2b" }, "algorithms": { "descriptors": { "descriptors": { "method": "fingerprint", "type": "MP2D" }, "similarity": { "method": "Algorithm::Similarity.tanimoto", "min": 0.1 }, "feature selection": null,</pre>		id	582b93e5ca78370057b50d2b		id	path	string
		subjectid			authorization token	header	string
		Response Messages					
		HTTP Status Co		Respons	se Model		ŀ
		200	OK Bad Barwart				
		400	Bad Request Unauthorized				
		403	Forbidden				
		404	Resource Not Found				
"prediction": {	Try it out!	Hide Response					
"method": "Algorithm::Cla }	issification.weighted_maj	iny it out:					
},	01.57.725.00.004	Curl					
Response Code							
200							
Response Headers							
<pre>{ "server": "nginx/1.10.2", "date": "Fri, 20 Jan 2017 14:1 "content-type": "application/j "content-length": "1505448", "connection": "keep-alive",</pre>	.8:24 GMT", son",						

Links

nano-lazar REST API GUI. Swagger UI based documentation for API visualization and interaction.

https://enm.in-silico.ch

- nano-lazar Swagger API definition file https://enm.in-silico.ch/api/api.json
- nano-lazar REST API services source code repository https://github.com/opentox/lazar-rest
- nano-lazar REST API services gem library https://rubygems.org/gems/lazar-rest
- nano-lazar REST API services Rubydocs gem library documentation http://www.rubydoc.info/gems/lazar-rest
- nano-lazar REST API issue tracker https://github.com/opentox/lazar-rest/issues
- lazar (source code) https://github.com/opentox/lazar
- Swagger framework for APIs http://swagger.io/
- Open API Initiative https://www.openapis.org/

References

"x-content-type-options": "nosniff", "access-control-allow-methods": "GET, POST, DELETE, PUT, PATCH, OPTIONS", "access-control-allow-credentials": "true", "access-control-allow-origin": "*", "access-control-allow-headers": "Origin, X-Requested-With, Content-Type, api_key, Authorization"

Figure 1: Swagger UI for the nano-lazar REST API

QMRF support

lazar-rest supports (Q)SAR Model Reporting Format (QMRF). The integrated QSAR-report library[4] generates QMRF reports in XML format with basic model information (e.g. validation results according to OECD guidelines). The QMRF report library is independent of other IST libraries (e.g. lazar, nano-lazar-gui, lazar-rest) and can be used by other applications that need QMRF reporting.

- [1] 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.
- [2] Andreas Maunz, Martin Gütlein, Micha Rautenberg, David Vorgrimmler, Denis Gebele, and Christoph Helma. Iazar: 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.
- [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, Christoph Helma, and Denis Gebele. qsar-report Ruby gem library, September 2016. URL https://doi.org/10.5281/zenodo.179038.
- [5] Barry Hardy, Nicki Douglas, Christoph Helma, Micha Rautenberg, Nina Jeliazkova, Vedrin Jeliazkov, Ivelina Nikolova, Romualdo Benigni, Olga Tcheremenskaia, Stefan Kramer, et al. Collaborative development of predictive toxicology applications. *Journal of cheminformatics*, 2(1):1, 2010. doi: 10.1186/1758-2946-2-7.

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