

# eNanoMapper - enabling systems biology for nanosafety

Egon Willighagen

Maastricht University, The Netherlands

@egonwillighagen

ORCID:0000-0001-7542-0286

*Systems Biology in Nanosafety Research*

*Stockholm, 9-10 November 2015*

*#nanosysbio*



**Maastricht University**

*Leading  
in Learning!*




# **(on behalf of...)**

These slides are mine and may not fully reflect the opinion of all partners.



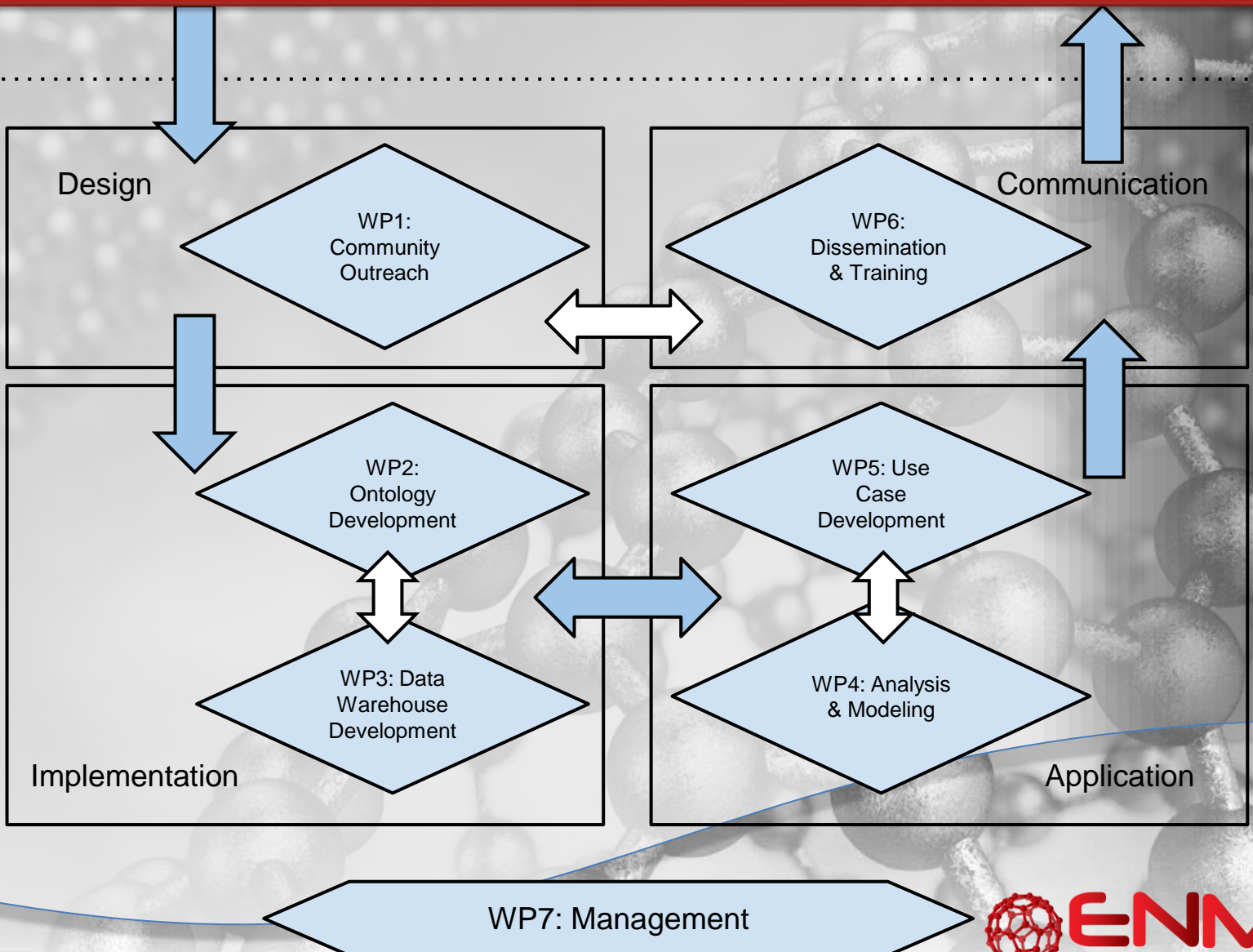
Douglas Connect  
Working communities



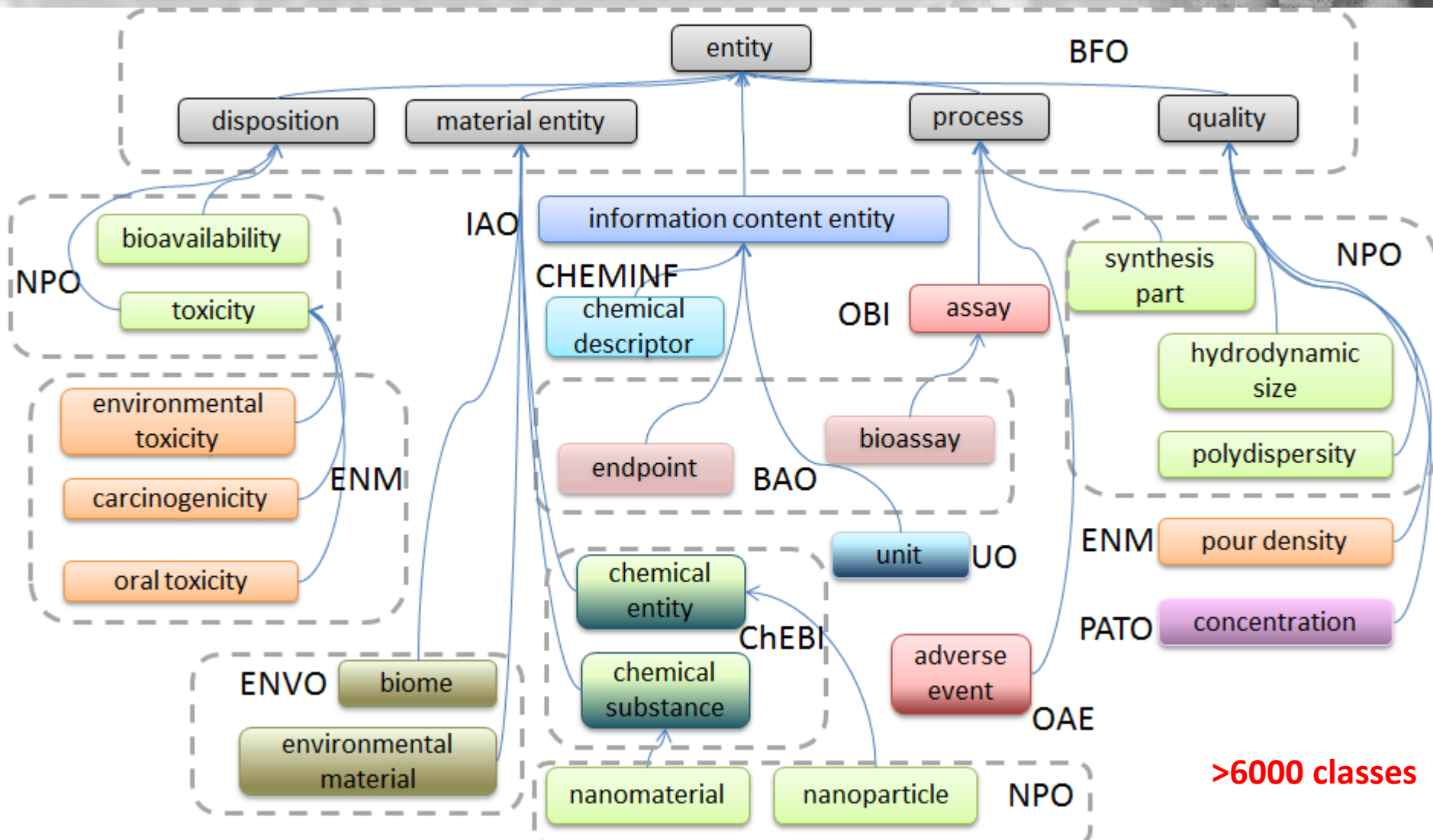
**!QFA**  
consult



# Workpackages



# Ontology assembled from multiple sources



# Excel Files (NanoSafety Cluster)

```

"SUBSTANCE_RECORD": {
  "COMPANY_UUID": {
    "COLUMN_INDEX": "A"
  },
  "PUBLIC_NAME": {
    "COLUMN_INDEX": "A"
  },
  "OWNER_NAME": {
    "ITERATION": "ABSOLUTE_LOCATION",
    "COLUMN_INDEX": "E",
    "ROW_INDEX": 3
  },
  "SUBSTANCE_TYPE": {
    "ITERATION": "JSON_VALUE",
    "JSON_VALUE": "Nanoparticle"
  },
  "EXTERNAL_IDENTIFIERS": [
    {
      "ID": {
        "COLUMN_INDEX": "D",
        "ITERATION": "ROW_SINGLE"
      },
      "TYPE": {
        "ITERATION": "ABSOLUTE_LOCATION",
        "COLUMN_INDEX": "D",
        "ROW_INDEX": 7
      }
    }
  ]
}

```

	A	B	C	D	E	F	G
1	Endpoint	Ca	Core comp	Surface mo	External Ide	Cell.association	
2	Protocol				ICP-AES		
3	Guideline				doi: 10.1021/nn4		
4	type_of_study						
5	type_of_method				ICP-AES		
6	data_gathe	Description			Perkin-Elmer		
7	Endpoint	Element	Abbreviate	Classificatio	Net cell associatio	Net cell ass	Net cell ass
8	Cell				A549	A549	A549
9	MEDIUM						
10	Condition						
11	Designation				Mean	SD	N
12	Units				mL/ug(Mg)	1/ug(Mg)	
13	G15.AC	[Au]	AC	Anionic	0.02751	0.01654	3
14	G15.AHT	[Au]	AHT	Cationic	0.49705	0.08013	3

Free text search

Showing 14 entries (1 to 14)

First Previous 1 Next Last

Free text search

size distribution

Entries

All ▾

Query expansion

without ▾

Search

JSON

Term ▾	Title ▾	Related to ▾	Hit importance ▾	Find studies ▾
<a href="#">PC_GRANULOMETRY</a>	Particle size distribution (Granulometry)	<a href="#">CHMO_0002119</a>	4.986	subclass
	<a href="#">OECD Guideline 110 (Particle Size Distribution / Fibre Length and Diameter Distributions)</a>	<a href="#">AGGLOMERATION_AGGREGATION</a>	4.986	by protocol
	<a href="#">OECD Guideline 110 (Particle Size Distribution / Fibre Length and Diameter Distributions)</a>	<a href="#">ASPECT_RATIO_SHAPE</a>	4.986	by protocol
	<a href="#">OECD Guideline 110 (Particle Size Distribution / Fibre Length and Diameter Distributions)</a>	<a href="#">CRYSTALLITE_AND_GRAIN_SIZE</a>	4.986	by protocol
	<a href="#">OECD Guideline 110 (Particle Size Distribution / Fibre Length and Diameter Distributions)</a>	<a href="#">PC_GRANULOMETRY</a>	4.986	by protocol
	<a href="#">ISO 15901-1:2005 with Cor 1:2007 (Pore size distribution and porosity of solid materials by mercury porosimetry and gas adsorption - Part 1: Mercury porosimetry)</a>	<a href="#">POROSITY</a>	4.986	by protocol
<a href="#">NPO_1694</a>	<a href="#">Particle size in media</a>	<a href="#">CRYSTALLITE_AND_GRAIN_SIZE</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE D10</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE D50</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE D90</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE DT95</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694</a>	<a href="#">PARTICLE SIZE DT99</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint
<a href="#">NPO_1694 NPO_1617</a>	<a href="#">Core size</a>	<a href="#">PC_GRANULOMETRY</a>	1.617	by endpoint

[Home](#)[Structure search](#)[All substances](#)[Import substance](#)[JSON](#)

## Help: Substances

Chemical substance, a material with a definite chemical composition. [REACH guide](#)

Mono-constituent ? and multi-constituent ? substances. Main constituent ? Additive ? Impurity ?

Composition

P-Chem (2)

Env Fate (3)

Eco Tox (4)

Tox (2)

Filter...

## TO\_BIODEG\_WATER\_SCREEN\_SECTION (3)

Name	Conditions	Effects		Interpretation	Protocol		
	Time Point	Endpoint	Result	Result	Guidance	Owner	UUID
Biodegradation in water: screening tests, IUC4#1/Ch.3.5	28 d	% Degradation	= 90%	-	OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	IUC4 TODO	IUC4-1d75f...
Biodegradation in water: screening tests.001	3 h	% Degradation	= 0%	readily biodegradable	OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	IUC4 TODO	IUC5-2ea8...
	7 d	% Degradation	= 20%				
	14 d	% Degradation	= 50%				
	28 d	% Degradation	= 85%				
Biodegradation in water: screening tests.002	3 h	% Degradation	= 9%	inherently biodegradable	N/A	IUC4 TODO	IUC5-69bc...
	7 d	% Degradation	= 40%				
	14 d	% Degradation	= 50%				
	28 d	% Degradation	= 80%				

Showing 1 to 3 of 3 entries

[Previous](#) [Next](#)

# Integration: Application Programming Interface (API)

## compound : Chemical structures search

[Show/Hide](#) | [List Operations](#) | [Expand Operations](#) | [Raw](#)

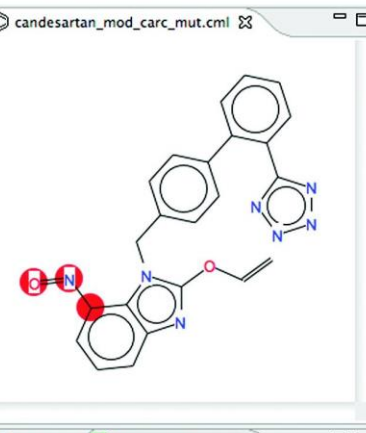
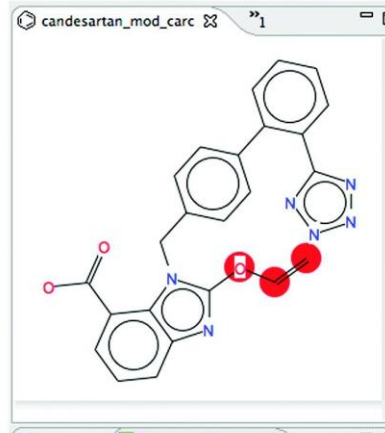
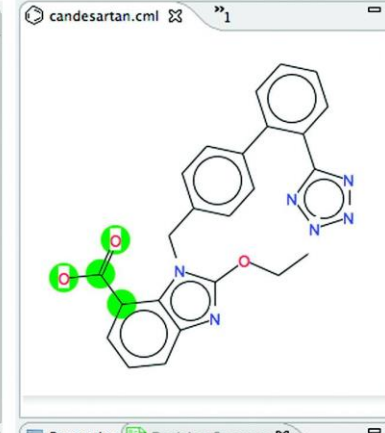
GET	/query/compound/{term}/{representation}	Exact compound search
GET	/query/similarity	Similarity search
GET	/query/smarts	Substructure search

## substance : Substance search

[Show/Hide](#) | [List Operations](#) | [Expand Operations](#) | [Raw](#)

GET	/query/substance/facet	Search substances by study owner
GET	/query/substance/reference	Search substances by reference structures
GET	/query/substance/related	Search substances by related structures
GET	/query/substance/study/experiment/{term}	Search substances by protocol application parameters
GET	/query/substance/study/owner/{term}	Search substances by study owner
GET	/query/substance/study/protocol/{term}	Search substances by study protocol parameters
GET	/query/study	Search endpoint summary

# Integration: Decision Support

(a)  (b)  (c) 

Properties Decision Support

- AHR
  - Carcinogenicity
    - CPDB Signature Alerts [1 pos]
      - [C]([C])(O)
    - CPDB Signature Significance [1 pos]
      - Result: 2.439
    - CPDB exact matches [no hits]
    - CPDB nearest neighbour [no hits]
  - Mutagenicity
    - Ames Signature Significance [1 pos]
      - [C](p[C]p[C])(N)
    - Ames Structural Alerts [1 pos]
      - Aromatic nitroso
    - Ames exact matches [no hits]
    - Ames nearest neighbour [no hits]

Bioclipse

File Edit Window Install Help

NanoTox

- 10.1002.smll.20120
- Al2O3.nmx
- list.nmx
- newMaterial.js
- test.js
- Test
- Virtual

NanoTox/Al2O3.nmx

Chemical Formula	Al2O3
Type	METALOXIDE
Zeta Potential	-24.0 eV

Ola Spjuth, et al.  
JCIM, 2011, doi:  
10.1021/ci200242c

# Systems Biology: Pathways

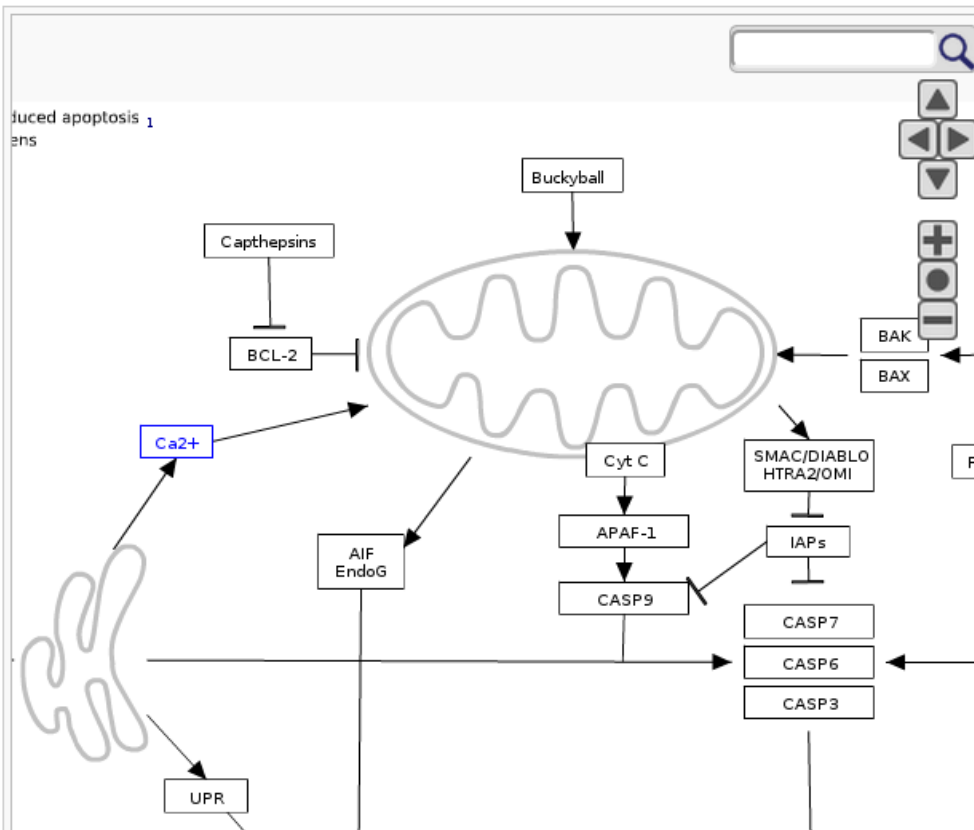
137.120.195.8 talk for this ip log in / create account



pathway discussion view source

## Nanomaterial induced apoptosis (Homo sapiens)

Egon Willighagen, Anwesha Bohler



### Buckyball

Annotated with: NPO\_730

(NanoParticle Ontology)

[Find pathways with Buckyball...](#)

Unable to load external references.


### Contents

[\[hide\]](#)


- [1 Curation](#)
- [Tags](#)
- [2](#)
- [Description](#)
- [3 Ontology](#)
- [Tags](#)
- [4](#)
- [Bibliography](#)
- [5 History](#)
- [6 External references](#)

# WikiPathways: capturing the full diversity of pathway knowledge

Martina Kutmon<sup>1,2,\*</sup>, Anders Riutta<sup>3</sup>, Nuno Nunes<sup>1</sup>, Kristina Hanspers<sup>3</sup>,  
Egon L. Willighagen<sup>1</sup>, Anwesha Bohler<sup>1</sup>, Jonathan Mélius<sup>1</sup>, Andra Waagmeester<sup>1,4</sup>,  
Sravanthi R. Sinha<sup>5</sup>, Ryan Miller<sup>1</sup>, Susan L. Coort<sup>1</sup>, Elisa Cirillo<sup>1</sup>, Bart Smeets<sup>1</sup>,  
Chris T. Evelo<sup>1,2</sup> and Alexander R. Pico<sup>3,\*</sup>

 Author Affiliations

 \*To whom correspondence should be addressed. Tel: +31 43 38 82913; Fax: +31 43 38 81996; Email: [martina.kutmon@maastrichtuniversity.nl](mailto:martina.kutmon@maastrichtuniversity.nl)

 Correspondence may also be addressed to Alexander R. Pico. Tel: +1 415 734 2741; Fax: +1 415 355 0960; Email: [apico@gladstone.ucsf.edu](mailto:apico@gladstone.ucsf.edu)

Received September 16, 2015.

Accepted September 28, 2015.

## Abstract

WikiPathways (<http://www.wikipathways.org>) is an open, collaborative platform for capturing and disseminating models of biological pathways for data visualization and analysis. Since our last NAR update, 4 years ago, WikiPathways has experienced massive growth in content, which continues to be contributed by hundreds of individuals each year. New aspects of the diversity and depth of the collected pathways are described from the perspective of researchers interested in using pathway information in their studies. We provide updates on extensions and services to support pathway analysis and visualization via popular standalone tools, i.e.

## This Article

Nucl. Acids Res. (2015)  
doi: 10.1093/nar/gkv1024

First published online: October 19, 2015

This article is Open Access

Abstract **Free**

» Full Text (HTML) **Free**


Full Text (PDF) **Free**


SUPPLEMENTARY DATA

 Classifications

 Services

 Responses

 Citing Articles

 Google Scholar

 PubMed

 ORCID

Profile for Riutta, A.  
<http://orcid.org/0000-0002-4693-0591>

Profile for Willighagen, E.  
<http://orcid.org/0000-0001-7542-0286>

Profile for Bohler, A.  
<http://orcid.org/0000-0001-7073-5852>

Profile for Mélius, J.  
<http://orcid.org/0000-0001-8624-2972>

Profile for Waagmeester, A.  
<http://orcid.org/0000-0001-9773-4008>

Profile for Sinha, S.

# WikiPathways: capturing the full diversity of

1. Select tissue of interest

2. Select pathway from table of tissue-specific results

3. View selected pathway with tissue expression data overlay

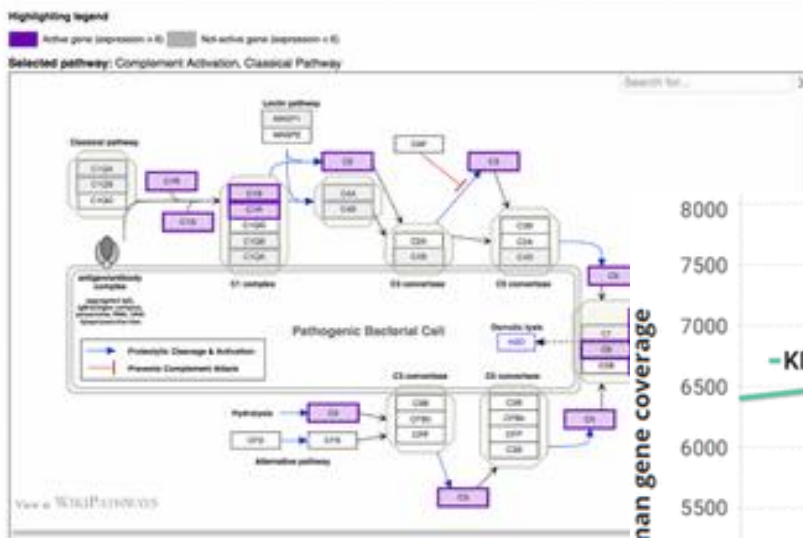
Select tissue:

☐ Show generic pathways

View all...

Gradient color scale: 0-3 3-6 6-7 7-10 >10

Pathways	Linkout	Median	Active genes	Measured genes	%
Felbamate Metabolism	WP2816	10.88	2	2	100
Cytidine Metabolic Pathway	WP2536	9.83	1	1	100
Lidocaine metabolism	WP2646	8.77	2	2	100
Nicotina Metabolism	WP1800	8.31	5	6	83
Polycy Pathway	WP690	7.23	3	4	75
Tamoxifen metabolism	WP681	7.22	12	21	57
Complement Activation, Classical Pathway	WP545	7.22	9	17	52
Diclofenac Metabolic Pathway	WP2491	7.21	2	4	50
Synthesis and Degradation of Ketone Bodies	WP311	6.94	3	5	60
Arachidonic Epoxide/Hydroxy Epoxide Hydrolyase	WP675	6.54	3	7	42
Benzodiazepine metabolism	WP696	6.49	4	9	44
Folate Alcohol and Cancer Pathway	WP1569	6.49	4	8	50
Phase I biotransformations, non P450	WP136	6.44	3	8	37
Complement and Coagulation Cascades	WP506	6.35	28	50	46
Glycine Metabolism	WP1495	6.21	1	3	33
Blood Clotting Cascade	WP272	6.18	8	24	33
Alanine and aspartate metabolism	WP106	6.08	9	12	41

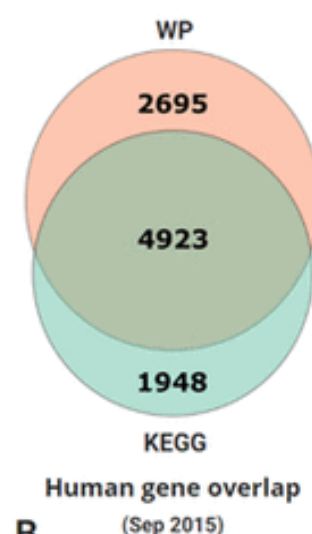
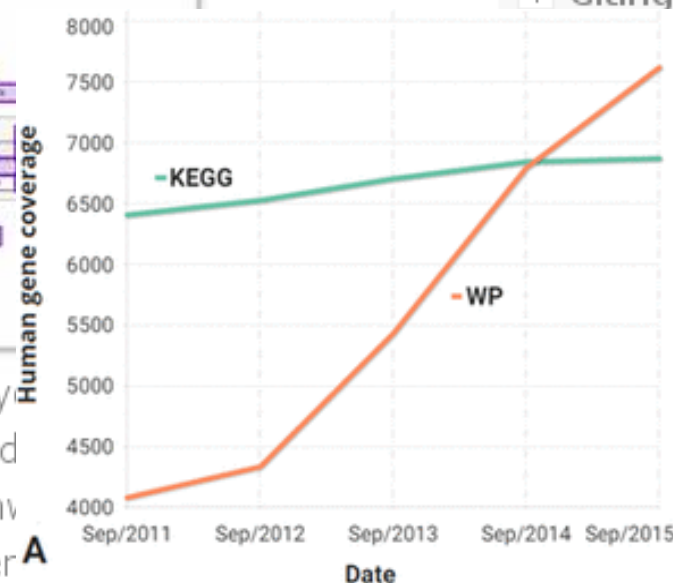


gmeester<sup>1,4</sup>,  
Smeets<sup>1</sup>,

3; Fax: +31 43

415 734 2741;

September 16, 2015.  
September 28, 2015.



## This Article

Nucl. Acids Res. (2015)  
doi: 10.1093/nar/gkv1024

First published online: October 19, 2015

This article is Open Access

Abstract **Free**

» Full Text (HTML) **Free**

Full Text (PDF) **Free**

SUPPLEMENTARY DATA

+ Classifications

+ Services

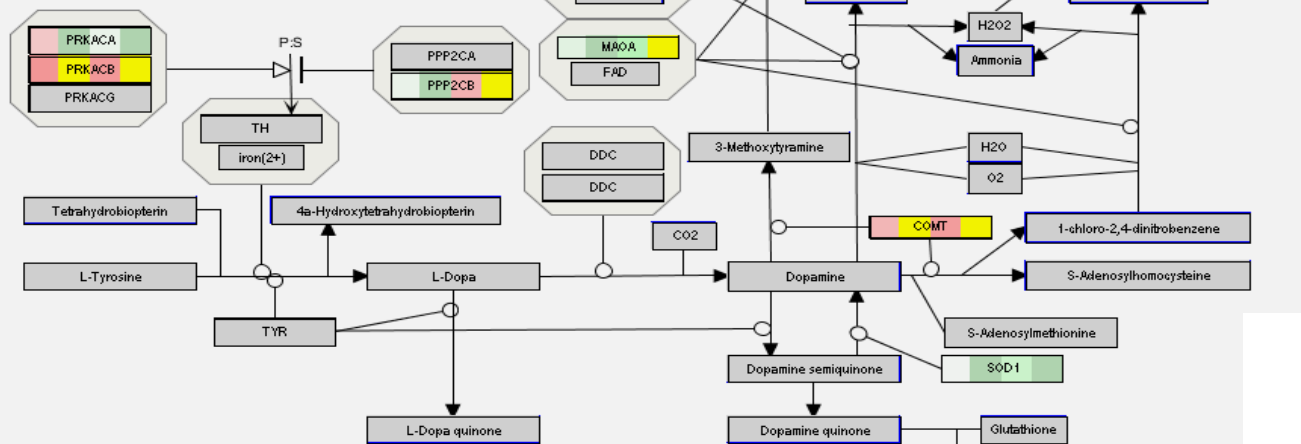
+ Responses

+ Citing Articles

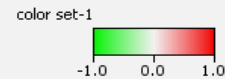
to be contributed by hundreds of individuals each year. The diversity and depth of the collected pathways are of great perspective of researchers interested in using pathway studies. We provide updates on extensions and server-based pathway analysis and visualization via popular standalone tools, i.e.

Profile for Sinha, S.

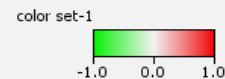
# Dopamine metabolism



P.Value.2 (color set-3)  
logFC.2 (color set-1)  
P.Value.025 (color set-2)  
logFC.025 (color set-1)



color set-2  
[P.Value.025] <= 0.05

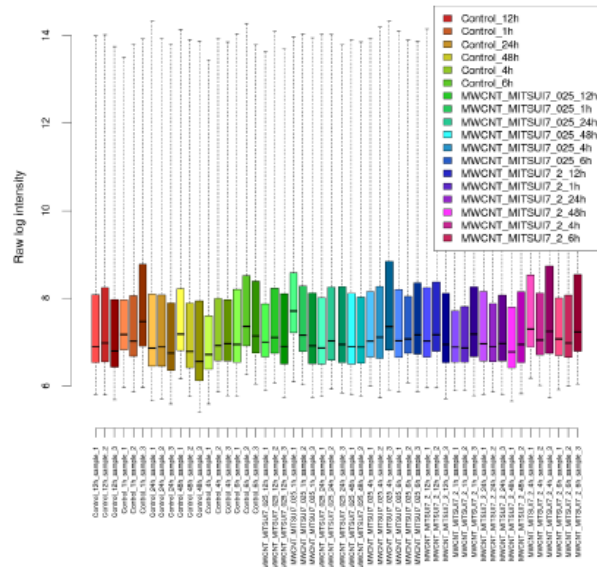


color set-3  
[P.Value.2] <= 0.05

Color rule not met  
No data found

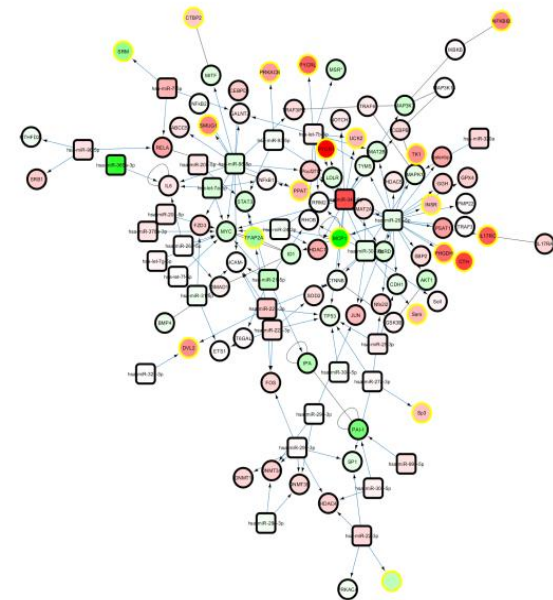
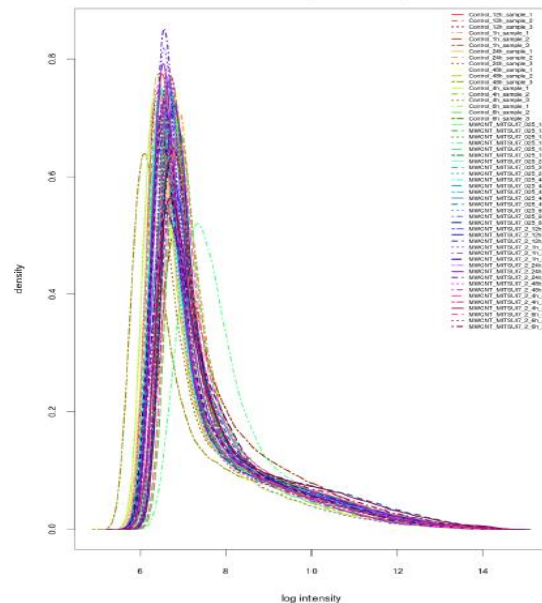
Boxplot of raw intensities

Distributions should be comparable between arrays



Density histogram of raw intensities

Curves should be comparable between arrays



RESEARCH

Open Access

# eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment

Janna Hastings<sup>1\*</sup>, Nina Jeliakova<sup>2</sup>, Gareth Owen<sup>1</sup>, Georgia Tsiliki<sup>3</sup>, Cristian R Munteanu<sup>4,5</sup>, Christoph Steinbeck<sup>1</sup> and Egon Willighagen<sup>6</sup>

## Abstract

Engineered nanomaterials (ENMs) are being developed to meet specific application needs in diverse domains of the engineering and biomedical sciences (e.g. drug delivery). However, accompanying the exciting proliferation of novel nanomaterials is a challenging race to understand and predict their possibly detrimental effects on human health and the environment. The eNanoMapper project ([www.enanomapper.net](http://www.enanomapper.net)) is creating a pan-European computational infrastructure for toxicological data management for ENMs, based on semantic web standards and ontologies. Here, we describe the development of the eNanoMapper ontology based on adopting and extending existing ontologies of relevance for the nanosafety domain. The resulting eNanoMapper ontology is available at [purl.enanomapper.net/ontology/enanomapper.owl](http://purl.enanomapper.net/ontology/enanomapper.owl). We aim to make the re-use of external ontology content seamless and thus we have developed a library to automate the extraction of subsets of ontology content and the subsets into an integrated whole. The library is available (open source) at <http://github.com/enanomapper/slimmer/>. Finally, we give a comprehensive survey of the domain content and identify gap areas. ENM safety boundary between engineering and the life sciences, and at the boundary between molecular granularity and granularity. This creates challenges for the definition of key entities in the domain, which we also discuss.

**Keywords:** Nanomaterial, Safety, Ontology

## Background

Nanomaterials are materials in which the individual components are sized roughly in the 1-100 nanometer range in at least one dimension, although an exact definition is still being debated [1,2]. Particles in this size range display special properties having to do with their very large ratio of surface area to volume [3]. Natural nanomaterials include viral capsids and spider silk. Recent years have seen an explosion in the development of engineered nanomaterials (ENMs) aiming to exploit the special properties of these materials in various domains including biomedicine (e.g. as vehicles for drug delivery), optics and electronics [3].

Counterbalancing the many possible benefits of nanotechnology, nanoparticles also pose risks to human and environmental health [4]. These dangers, regulatory bodies are calling attention and thorough toxicological and safety information into ENMs with the objective of feeding into predictive tools which are able to assist in redesigning safe nanomaterials. Evaluating the possible dangers of different nanomaterials assembling a wealth of information on those the composition, shape and properties of the nanoparticles, their interactions with biology across different tissues and species, and their behaviour into the natural environment. This arising from different disciplines with high needs requirements, methods, labelling and practices. Regulatory descriptions of ENMs those needed for nanoQSAR analyses. Safety may also vary under different conditions

\*Correspondence: [hastings@ebi.ac.uk](mailto:hastings@ebi.ac.uk)

<sup>1</sup>European Molecular Biology Laboratory – European Bioinformatics Institute (EMBL-EBI), Cambridge, United Kingdom

Full list of author information is available at the end of the article



© 2015 Hastings et al.; licensee BioMed Central. This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution in any medium, provided the original work is properly credited. The Creative Commons Public Domain Dedication waiver (<http://creativecommons.org/publicdomain/zero/1.0/>) applies to the data made available in this article, unless otherwise stated.



BEILSTEIN JOURNAL OF NANOTECHNOLOGY

## The eNanoMapper database for nanomaterial safety information

Nina Jeliakova<sup>1\*</sup>, Charalampos Chomenidis<sup>2</sup>, Philip Doganis<sup>2</sup>, Bengt Fadeel<sup>3</sup>, Roland Grafström<sup>3</sup>, Barry Hardy<sup>4</sup>, Janna Hastings<sup>5</sup>, Markus Hegi<sup>4</sup>, Vedrin Jeliakova Nikolay Kochev<sup>1,6</sup>, Pekka Kohonen<sup>5</sup>, Cristian R. Munteanu<sup>7,8</sup>, Haralambos Sarimvee Bart Smeets<sup>7</sup>, Pantelis Sopasakis<sup>2,9</sup>, Georgia Tsiliki<sup>2</sup>, David Vorgrimmler<sup>10</sup> and Egon Willighagen<sup>7</sup>

## Full Research Paper

**Address:**  
<sup>1</sup>Ideaconsult Ltd., Sofia, Bulgaria, <sup>2</sup>National Technical University of Athens, School of Chemical Engineering, Athens, Greece, <sup>3</sup>Norvinska Institutet, Stockholm, Sweden, <sup>4</sup>Douglas Connect GmbH, Zeiningen, Switzerland, <sup>5</sup>European Molecular Biology Laboratory – European Bioinformatics Institute (EMBL-EBI), Hinxton, United Kingdom, <sup>6</sup>Department of Analytical Chemistry and Computer Chemistry, University of Plovdiv, Plovdiv, Bulgaria, <sup>7</sup>Department of Bioinformatics, NUTRIM, Maastricht University, Maastricht, The Netherlands, <sup>8</sup>Computer Science Faculty, University of A Coruña, A Coruña, Spain, <sup>9</sup>IMT Institute for Advanced Studies Lucca, Lucca, Italy and <sup>10</sup>In silico toxicology GmbH (IST), Basel, Switzerland

**Email:**  
Nina Jeliakova<sup>\*</sup> - [jeliakova.nina@gmail.com](mailto:jeliakova.nina@gmail.com)

<sup>\*</sup> Corresponding author

**Keywords:**  
database; EU NanoSafety Cluster; nanoinformatics; nanomaterials; nanomaterials ontology; NanoQSAR; safety testing

## Abstract

**Background:** The NanoSafety Cluster, a cluster of projects funded by the European Commission, identified the need for a national infrastructure for toxicological data management of engineered nanomaterials (ENMs). Ontologies, open standards, and operable designs were envisioned to empower a harmonized approach to European research in nanotechnology. This provides a number of opportunities and challenges in the representation of nanomaterials data and the integration of ENM information originating from diverse systems. Within this cluster, eNanoMapper works towards supporting the collaborative safety management for ENMs by creating a modular and extensible infrastructure for data sharing, data analysis, and building computational tools for ENMs.

**Results:** The eNanoMapper database solution builds on the previous experience of the consortium partners in supporting data through flexible data storage, open source components and web services. We have recently described the design

# Library

Tsiliki et al. *J Cheminform* (2015) 7:46  
DOI 10.1186/s13321-015-0094-2



## RESEARCH ARTICLE

## Open Access



# RRegrs: an R package for computer-aided model selection with multiple regression models

Georgia Tsiliki<sup>1\*</sup>, Cristian R. Munteanu<sup>2,3†</sup>, Jose A. Seoane<sup>4</sup>, Carlos Fernandez-Lozano<sup>2</sup>, Haralambos Sarimvee<sup>1</sup> and Egon L. Willighagen<sup>1</sup>

## Abstract

**Background:** Predictive regression models can be created with many different modelling approaches. Choices need to be made for data set splitting, cross-validation methods, specific regression parameters and best model criteria, as they all affect the accuracy and efficiency of the produced predictive models, and therefore, raising model reproducibility and comparison issues. Cheminformatics and bioinformatics are extensively using predictive modelling and exhibit a need for standardization of these methodologies in order to assist model selection and speed up the process of predictive model development. A tool accessible to all users, irrespective of their statistical knowledge, would be valuable if it tests several simple and complex regression models and validation schemes, produce unified reports, and offer the option to be integrated into more extensive studies. Additionally, such methodology should be implemented as a free programming package, in order to be continuously adapted and redistributed by others.

**Results:** We propose an integrated framework for creating multiple regression models, called RRegRs. The tool offers the option of ten simple and complex regression methods combined with repeated 10-fold and leave-one-out cross-validation. Methods include Multiple Linear Regression, Generalized Linear Model with Stepwise Feature Selection, Partial Least Squares regression, Lasso regression, and Support Vector Machines Recursive Feature Elimination. The new framework is an automated fully validated procedure which produces standardized reports to quickly oversee the impact of choices in modelling algorithms and assess the model and cross-validation results. The methodology was implemented as an open source R package, available at <https://www.github.com/enanomapper/RRegrs>, by reusing and extending on the caret package.

**Conclusion:** The universality of the new methodology is demonstrated using five standard data sets from different scientific fields. Its efficiency in cheminformatics and QSAR modelling is shown with three use cases: predictive data for surface-modified gold nanoparticles, nano-metal oxides descriptor data, and molecular descriptors for acute aquatic toxicity data. The results show that for all data sets RRegRs reports models with equal or better performance for both training and test sets than those reported in the original publications. Its good performance as well as its adaptability in terms of parameter optimization could make RRegRs a popular framework to assist the initial exploration of predictive models, and with that, the design of more comprehensive in silico screening applications.

**Keywords:** Multiple regression, QSAR, R package, Caret-based tool

\*Correspondence: [tsiliki@central.rug.nl](mailto:tsiliki@central.rug.nl)

<sup>†</sup>Georgia Tsiliki and Cristian R. Munteanu contributed equally to this work

<sup>1</sup>School of Chemical Engineering, National Technical University of Athens,

91079 Polytechnic Street, Zografou Campus, 15701 Athens, Greece

Full list of author information is available at the end of the article

# NSC Newsletter Autumn 2015

## News from the NSC Projects

### eNanoMapper Updates and its Collaborations with the Community

**Authors:** Egon Willighagen, Friederike Ehrhart, Linda Rieswijk, Nina Jeliaskova, Chris Evelo, Lucian Farcas, Barry Hardy, Haralambos Sarimveis

License: CC-BY 4.0



February this year marked the completion of the first draft versions of three key components of the eNanoMapper platform: the database, ontology and modelling software. This update highlights these three contributions to the community and some of their applications to solve community challenges. Furthermore, we briefly discuss our new Associate Partner program and other outreach and dissemination activities.

Database - software and demonstration server: <http://data.enanomapper.net/>

The database software was recently described in detail in a publication in the Beilstein Journal of Nanotechnology (Jeliaskova et al., 2015), extending on the conference paper for the nanoinformatics symposium in Belfast in 2014 (Jeliaskova et al., 2014). These papers describe the database functionality, demonstrate the default graphical user interfaces (see Figure 1), focusing on the data formats supported to import nanosafety data, and the Application Programming Interface (API). The import and upload functionality currently supports a variety of NanoSafety cluster Excel templates, OECD HT (IUCLID .isz files) and a custom RDF format for importing NanoWiki. ISA-Tab-Nano import and export is under active development. Furthermore, the importer can easily be extended to support more spreadsheet formats and templates, using the configurable parser with specific JSON configuration developed in the

# Acknowledgments

- **All eNanoMapper partners**
- **OpenTox - NM - Bioclipse integration**
  - dr Nina Jeliaskova (IdeaConsult Ltd.)
  - dr Ola Spjuth (Uppsala University, GenettaSoft)
- **WikiPathways project**
  - Prof. Alex Pico's team, UCSF
- **UM team and students**
  - Bart Smeets, Freddie Ehrhart, Linda Rieswijk, Marloes Poort, Lars Eijssen, Tina Kutmon, Ryan Miller, Anwasha Dutta, Prof. Chris Evelo

# FP7-eNanoMapper

## **"eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment"**

- Grant Agreement: 604134
- Duration: 36 months (1 Feb 2014 – 31 Jan 2017)