



# DELIVERABLE REPORT D6.6

## eNanoMapper Final Dissemination Report

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# 1. EXECUTIVE SUMMARY

The key objectives of WP6 are to disseminate and raise awareness of the scientific results, tools and applications developed in the eNanoMapper project among the user communities in academia and industry, and to provide training on these eNanoMapper tools, through online seminars, tutorials, and training events (workshops). In the third year of the project, the partners have produced a series of tutorials on tools developed in the technical workpackages and organized several workshops including the nanoEHS workshop in the context of the US-EU nanoEHS platform. Project members actively participated in numerous conferences including the EUROTOX congress in Sevilla, Spain, and the OpenTox conference in Rheinfelden, Germany, and several eNanoMapper presentations are scheduled for the joint nanosafety conference in Malaga in February 2017. We also organized the 2nd Nanosafety Forum for Young Scientists in Visby, Sweden, with the EU nanosafety cluster. The eNanoMapper project is well represented in the NanoSafety Cluster as WG4 (databases) was chaired by Egon Willighagen (UM) and now by Nina Jeliakova (IDEA) and WG8 (systems biology) is chaired by Bengt Fadeel (KI) while Barry Hardy (DC) co-chairs the working group on databases & computational modeling in the US-EU nanoEHS platform. Overall, dissemination and training activities in the project accelerated in the third and final year, as planned, and all project partners actively contributed to community development.

## 2. INTRODUCTION

WP6 is concerned with the effective dissemination and development of news, findings, progress, lessons learned, practices, resources and services created, scientific discoveries and inventions from the eNanoMapper project. The focus of the activities has revolved around the engagement of user communities who use the applications developed in the other workpackages in the project. The project has provided guidance and training both through online tutorials and meetings and through face-to-face workshops and conferences. The active use of hands-on scientific exercises and problem-solving in both virtual and face-to-face workshops pursued in community development activities in recent years for instance in OpenTox has been extended to develop active and engaged groups of users for eNanoMapper. Advances in state-of-the-art pursued by the project in integrated data analysis and modelling have been disseminated through scientific publications and conference presentations. The

activities of WP6 were coordinated closely to support the community outreach activities of WP1, in addition to developing outreach to new communities and users. Considerable emphasis has been placed on developing and disseminating effective solutions to other nanosafety cluster projects, eg., NANoREG.

## 2.1 LIST OF DELIVERABLES

During the third year of the project, the deliverable on eNanoMapper tutorials has been finalized (D6.3) and additional deliverables are due at the end of the project, including reports on community development and exploitation, as seen in the table below. The community development work within eNanoMapper (D6.4, due Month 36) is focused on the development of user communities and the implementation of eNanoMapper resources and applications, through the EU nanosafety cluster and also through the US-EU nanoEHS [environmental health & safety] platform. This work builds on the work on community outreach in WP1. The exploitation work, in turn, is aimed at delivering a business model and exploitation plan to maintain the impact of the project beyond the life-time of the funded project (D6.5, due Month 36).

| Deliverable                                   | Lead Beneficiary | Delivery Month |
|---|------------------|----------------|
| D6.1 eNanoMapper Year 1 Dissemination Report  | KI               | M12            |
| D6.2 eNanoMapper Year 2 Dissemination Report  | KI               | M24            |
| D6.3 eNanoMapper Tutorials                    | DC               | M33            |
| D6.4 eNanoMapper Community Development Report | DC               | M36            |
| D6.5 eNanoMapper Exploitation Report          | DC               | M36            |
| D6.6 eNanoMapper Final Dissemination Report   | KI               | M36            |

## 3. DISSEMINATION AND TRAINING

### 3.1 COMMUNITY WEBSITE

The creation of online tools in order to facilitate the communication and information exchange within the project and with the public and with other stakeholders was part of Task 6.1 and, hence, a public website ([www.enanomapper.net](http://www.enanomapper.net)) was launched at the beginning of the project and it has been further developed in order to build the library updated with all events, publications, presentations, posters, webinars, tutorials and public reports released by the consortium. In the recent period, a dedicated entry point for different applications developed in the project was created: <http://www.enanomapper.net/applications>, as well as 'one-stop' page showcasing results of the FP7 modelling projects (eNanoMapper, nanoPUZZLES, PRENANOTOX, MODERN, MEMBRANE-NANO-PART, MOD-ENP-TOX): <http://www.enanomapper.net/projects/>.

In addition, eNanoMapper has disseminated information about project activities and resources through the EU nanosafety cluster newsletter including the "winter" issue (No. 8, 2016) which included a section entitled *Spotlight on eNanoMapper* with 5 pages on eNanoMapper activities, eg., workshops and conferences organized by the project ([www.nanosafetycluster.eu](http://www.nanosafetycluster.eu)). We also provided an updated description of eNanoMapper to the 2016 edition of the EU cluster compendium.

eNanoMapper has also supported the CompNanoTox initiative (i.e., joint conferences of the nanosafety modeling projects), by creating the webpages for the conferences in 2015 (Malaga, Spain) (see 2nd dissemination report) and 2017 (Gdansk, Poland): <http://compnanotox2017.eu/>.

The eNanoMapper website was extended with two subdomains used as support tools in US-EU nanoEHS community activities (web-tools are presented in detail in section 3.4.2 in Deliverable 5.7):

- <https://nanoehs.enanomapper.net/> used for the US-EU NanoEHS scrimmage, June 2016, Arlington, USA

- <https://summit.enanomapper.net/> used for the 2016 EU-US NanoEHS workshop, October 2016, Rheinfelden, Germany



## NanoEHS Scrimmage

[About the Scrimmage](#) [Scenario A - Silver](#) [Scenario B - Copper](#) [Resources](#)

### Resources for participants

This nanoEHS Scrimmage event will enlist two sets of teams to compete in scientifically addressing hypothetical scenarios involving nanoscale pesticides. One will examine a nanoscale silver pesticidal product and one a nanoscale copper pesticidal product. There are many similarities in terms of their metallic nature and probable modes of action, and both have a reasonable body of literature to support the respective spill scenarios.



#### Scenario A: Daysville River Spill

The hypothetical pesticide product Nano-[Ag]-cide®, has been released in the Days River through an accidental spill of a large shipment of an aqueous suspension of the nanoform pesticide.

[VIEW SCENARIO A](#)



#### Scenario B: Daysville Road/Loading Dock Spill

A significant quantity of copper-based hypothetical pesticide product, Nano-[Cu]-cide®, has been released in powdered form near a loading dock onto an urban street.

[VIEW SCENARIO B](#)



#### Resources

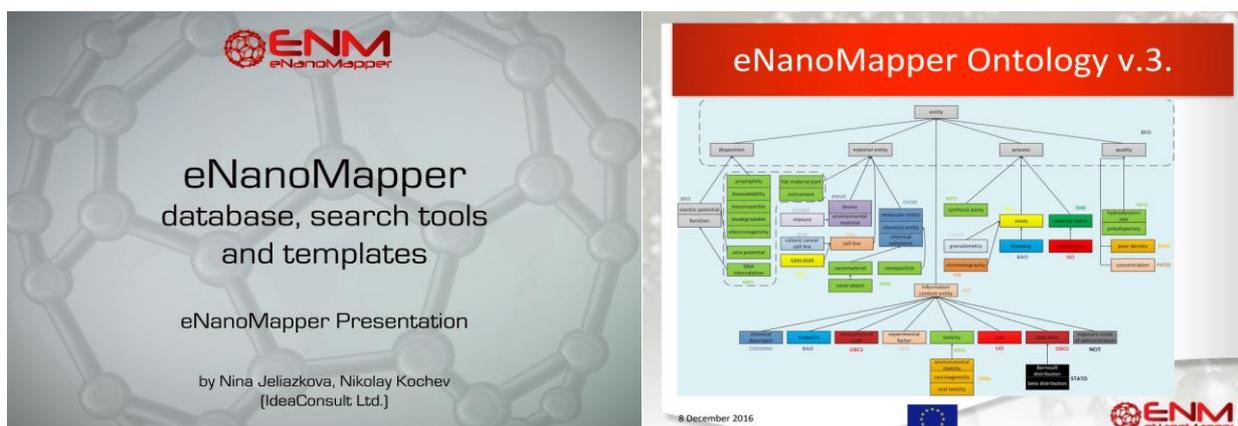
A collection of supporting information gathered and developed so that participants have a robust set of reference resources to utilize for the scrimmage and related actions.

[EXPLORE RESOURCES](#)

### 3.2 VIRTUAL SEMINARS

Webinars on topics related to eNanoMapper research and innovation activities, scientific applications, and case studies were held during the project using a virtual conferencing facility linked to the project website: <http://www.enanomapper.net/library/webinars>. During the recent project period, the following webinars on database solutions and ontologies, respectively, took place:

- November 17, 2016: [eNanoMapper Database, Search Tools and Templates](#) (Nina Jeliaskova, IDEA). The presentation is publicly available at: <http://www.enanomapper.net/library/db-search-templates>
- December 8, 2016: [eNanoMapper Ontology Presentation + Discussion on Sustainability](#) - (Linda Rieswijk, UM). The presentation is publicly available at: <https://nciphub.org/resources/2001>



### 3.3 WORKSHOPS AND PRESENTATIONS

The eNanoMapper consortium has organized numerous workshops throughout the project in order to promote advances in areas covered by eNanoMapper and to foster collaborations and common approaches with other projects in the EU nanosafety cluster and beyond, including a series of events during the third and final year, including hands-on workshops as well as the young scientist forum. The project is also involved in the joint nanosafety conference in Malaga in 2017 (see below) and project members have actively participated in international conferences with oral or poster presentations (about one dozen poster presentations prepared during the third year).

#### **1. Hands-On Workshop on Nano Safety Assessment, Basel, Switzerland, February 10, 2016.**

This event, organized back-to-back with the annual consortium meeting, brought together input and approaches from several EU projects, including eNanoMapper, NanoFASE, GUIDENANO, SUN.



#### **OBJECTIVES**

- To work through nanotechnology safety examples and exercises using existing data resources and modelling tools;
- To use information in support of nanotechnology risk assessment goals and to discuss current results;
- To discuss the role of harmonisation and ontology in the use of multiple modelling and assessment tools applied to nanosafety.

The workshop focused on specific cases and practical examples in which the group worked through modelling, analysis and assessment exercises, and discussed the results. All materials used during the event are publicly available:

<http://www.enanomapper.net/events/workshop-basel-2016/program>

The programme included interactive sessions, with available tutorials, guidance and exercises materials provided in advance to participants, as follow:

- **Nano Safety Science & Assessment**, Barry Hardy (Douglas Connect / eNanoMapper) and Vladimir Lobaskin (UCD)
- **Entering and Analysing Nano Safety Data**, Egon Willighagen (University of Maastricht) and Nina Jeliaskova (Ideaconsult / eNanoMapper)
  - *Workshop participants worked through the preparation of datasets to be used for modelling and risk assessment. The combination of data from multiple sources using common harmonised ontology and templates were carried out by the group.*
- **Data Requirements for Nanotoxicity Read Across Predictions**, Christoph Helma (in silico toxicology / eNanoMapper)
  - *Data requirements for nanotoxicity read across predictions and the coverage of currently available datasets were presented and discussed. Participants were able to evaluate a prototype nanoparticle read across application and provide feedback for future developments.*
  - *Guidance: Nano-Lazar Toxicity Predictions*
- **Bioinformatics Analysis of Nanotechnology-based Omics Data**, Pekka Kohonen and Penny Nymark (Misvik Biology / eNanoMapper)
  - *Bioinformatics analysis of an omics dataset generated on a nanoparticle category will be carried out and the dose-dependence and mechanistic interpretations discussed.*
  - *Guidance: Tutorial | Data*
- **Developing Nano-QSAR predictive toxicology models**, Philip Doganis and Haralambos Sarimveis (NTUA / eNanoMapper)
  - *The group worked on developing nanoQSAR models based on data available from the data.enanomapper.net server and using the eNanoMapper computational infrastructure. Demonstrate how a modeler can use diverse sets of nanoparticle descriptors, including descriptors derived from protein-corona information.*
  - *Guidance: pdf | 11\_00 Developing Nano-QSAR predictive toxicology models.xml*
- **Modelling Nano Exposure**, Claus Svendsen (UK Natural Environment Research Council / GUIDEnano and NanoFASE) and Wouter Fransman (TNO / GUIDEnano)
  - *The participants worked through the modelling of two exposure scenarios **a)** human (occupational and consumer) exposure to nanoparticles across different scenarios in the lifecycle of a product, and **b)** life cycle analysis of nanoparticles in the environment.*
  - *Guidance: NECID Guidance | Stoffenmanager Nano | Case 1 | Case 2 | Exercise Soil | Exercise River*
- **Nano Risk Assessment**, Fadri Gottschalk (ETSS / SUN)

- *The participants worked through a risk assessment example combining hazard and exposure data. The participants will be familiarized with stochastic modeling and uncertainty analysis software with focus on environmental exposure, ecotoxicological effects and risks in the context of emerging materials such as engineered nanoparticles.*

## **2. 2<sup>nd</sup> eNanoMapper Ontology Hackathon/Workshop, Leiden, The Netherlands, March 3, 2016**

The 2nd eNanoMapper Ontology hackathon/workshop was organized on March 3, 2016 in Leiden, The Netherlands. The event was hosted by TNO and Wouter Fransman (TNO) provided the opening remarks. The following lectures and tutorials were presented at the workshop:

- Lecture 1 - A general introduction to semantic web and ontology, benefit of using ontologies in modern databases (Egon Willighagen, UM)
- Lecture 2 - the eNanoMapper ontology - an explanation of the specific concept, intention and function of the eNanoMapper ontology, adoption of 3rd party content (Gareth Owen, EMBL-EBI)
- Lecture 3 - ISA-TAB/ISA-TAB-Nano and the new ISA-JSON specification. Java classes, mapping to the eNanoMapper data model (Nikolay Kochev, IDEA)
- Tutorial 1 - How to browse ontologies on online repositories like BioPortal or AberOwl, how to download ontologies and look up identifiers, how to download and browse ontologies with the open-source Protégé software (Linda Rieswijk / Freddie Ehrhart, UM)
- Tutorial 2 - Configurable parser for Excel templates. Creating JSON configuration for NanoSafety cluster templates (Nikolay Kochev, IDEA)
- Tutorial 3 - External validation: mapping coverage reports (Egon Willighagen, UM)

This was followed by the Hackathon (issues included: mapping NECID [Nano Exposure and Contextual Information Database] terms to ontology), and a general discussion on:

- what is needed to make ENM more interoperable for your database?
- how to improve the ENM? (data modelling etc.)
- what are your goals / your recommendations for technical developments or tools for interoperability

### 3. Workshop on Web Services for Computational Nanotoxicology, Athens, Greece, March 17, 2016

This Workshop aimed to test and strain the current in-development-state services in order to enable our team to fine-tune them for better performance. There were 20 participants from NTUA.

Website: [http://www.chemeng.ntua.gr/labs/control\\_lab/workshop.html](http://www.chemeng.ntua.gr/labs/control_lab/workshop.html). Program:

1. **Introduction to Computational Nanotoxicology.** Haralambos Sarimveis.
2. **eNanoMapper Modelling services.** Philip Doganis.
3. **Testing the services.** Charalampos Chomenidis, Georgios Drakakis, Georgia Tsiliki.

### 4. Hackathon on Ontology for Modelling & Nano-Descriptors, Athens, Greece, April 11, 2016

[http://www.chemeng.ntua.gr/labs/control\\_lab/2016hackathon.html](http://www.chemeng.ntua.gr/labs/control_lab/2016hackathon.html)

This hackathon worked on incorporating nanomaterial modelling terms into the eNanoMapper Ontology. There were 15 participants with physical or online presence from eNanoMapper (NTUA, EBI, UM), National Hellenic Research Foundation, and from the FP7- project, GuideNano.

The program included opening remarks by Haralambos Sarimveis (NTUA) and presentations by Egon Willighagen on "Introduction to ontologies and data integration", and Gareth Owen on "Introduction to the eNM ontology", and a tutorial by Linda Rieswijk & Freddie Ehrhart: "Tutorial: How to map terms to ontologies". The afternoon session was devoted to the Hackathon, and a follow-up.

The tutorial can also be found on the webpage: <http://enanomapper.net/library/browsing-ontology>

### 5. US-EU NanoEHS CoRs Workshop and Scrimmage, Arlington, USA, June 6-7, 2016

The 5th annual face to face workshop for the U.S –E.U. nanoEHS Communities of Research (CoRs) was held on 6-7 June, in Arlington, Virginia, USA. The workshop brought together the U.S.-EU Communities of Research (CoR), which are a platform for scientists to develop a shared repertoire of protocols and methods to overcome research gaps and barriers and to address environmental, health, and safety questions about nanomaterials. The goal of this workshop was to publicize progress towards CoRs goals and objectives, clarify and communicate future

plans, share best practices, and identify areas of cross-community collaboration. eNanoMapper team offered support in preparation of the scrimmage (concept, resources, etc.), prepared a web-tool (<https://nanoehs.enanomapper.net/>) used before, during and after the scrimmage, as well as participated actively at the event in Arlington.



## 6. Nano Korea 2016, Seoul, Korea, July 13-14, 2016

The Nano Korea conference, co-hosted by the Ministry of Science, ICT & Future Planning and the Ministry of Trade, Industry & Energy, included a satellite session on "Practical Hands-on Workshop on NanoSafety Assessment" <http://sympo.nanokorea.or.kr/2016/eng/sub2/05.php>. This session focused on specific cases and practical examples in which the group worked through modelling, analysis and assessment exercises, and discuss the results, and included also the presentations:

- Nanoinformatics for Safety, Standardization, and Regulation of Nanotechnologies (Nina Jeliaskova, IDEA)
- Risk Assessment of Manufactured Nanomaterials (Barry Hardy, DC)

The lectures were followed by two hands-on workshops:

- Data management: Entering and Analysing Nano Safety Data (Nina Jeliaskova, IDEA)
- Data modelling: Image descriptor calculation web tool (Barry Hardy, DC)



## 7. 2<sup>nd</sup> Nanosafety Forum for Young Scientists, Visby, Sweden, September 15-16, 2016.

Organizer: KI (chair: Bengt Fadeel): <http://www.enanomapper.net/events/young-scientists-forum>

The second edition of the Nanosafety Forum for Young Scientists took place in Visby on the island of Gotland (Sweden) on September 15-16, 2016. The meeting was organized by the eNanoMapper project in close collaboration with all the working groups in the EU Nanosafety Cluster and served as a forum for young scientists in EU-funded and some national nanosafety projects to interact and to present their work. The first meeting took place on Sicily in 2014 and it was decided early on to maintain the 'island concept', which is why the meeting was held on Gotland.

The meeting was chaired by Bengt Fadeel, Karolinska Institutet, Stockholm. A scientific committee consisting of the working group chairs in the EU Nanosafety Cluster reviewed all the submitted abstracts in a blinded fashion, and oral or poster presentations were awarded accordingly.



About 60 participants attended the meeting including 50 young scientists (students, post docs, and others) along with the two keynote speakers as well as several working group chairs from the EU Nanosafety Cluster, who served as session chairs. Prof. Iseult Lynch (Birmingham) presented the opening lecture, providing a broad overview of recent nanosafety research while prof. Roland Stauber (Mainz) presented the closing lecture, focusing on novel and intriguing aspects of nanoparticle-microbe interactions. The main part of the 2-day meeting was devoted to short oral presentations by young scientists (12 minutes per talk) as well as poster presentations. The scientific quality as well the quality of the actual presentations was excellent and a strong testament not only to the excellence of the young scientists, but also proof that the field of nanosafety research has progressed significantly in recent years. The discussions were animated.

The meeting was organized into several sessions, covering topics such as nanomaterial production and characterization, hazard assessment, modeling and systems biology,

environmental fate and behavior, and exposure assessment. The scientific committee, plus the project officer, Dr. Nicolas Segebarth of the European Commission, selected 3 oral presentations and 1 poster presentation for 'best oral/poster' awards. During the meeting, Egon Willighagen (UM) conducted an exercise with the participants on the ontology-based annotation of their abstracts (see Deliverable Report D3.3).

In addition to the scientific program, the participants also joined a guided tour of the Gotland Museum with its world-famous picture stones and a tour of the Medieval City of Visby, a UNESCO World Heritage Site, and a banquet at Gotland Museum. The Governor of Gotland County, Dr. Cecilia Schelin Seidegård, was the guest of honor at the banquet. The aim is to follow up on this event with a third meeting for young scientists in nanosafety research in the Fall 2018, possibly in Malta.

## **8. eNanoMapper Hands-on Workshop, Athens, Greece, September 29-30, 2016.**

Organizer: National Technical University of Athens (FP7-eNanoMapper).

Web: <http://www.enanomapper.net/events/hands-on-workshop-athens>

During this workshop, eNanoMapper partners described specific cases and practical examples in which the group worked through modelling, analysis and assessment exercises, and discuss the results.



## BACKGROUND

Computational modelling and software tools are increasingly important to support experimental testing and risk assessment in modern nanotoxicology. The EU has given particular emphasis in funding the development of computational methods for toxicological risk assessment of engineered nanoparticles.

- Modular infrastructure for data storage, sharing and searching, based on open standards and semantic web technologies, minimum information standards and established security solutions;
- Development of ontologies for the categorisation and characterisation of engineered nanomaterials in collaboration with other projects;
- Development of computational infrastructure for eNanoMapper toxicity modelling and prediction which may process all data made available through eNanoMapper (e.g., using algorithms available from the FP7-OpenTox project or statistical/data mining software).

As the eNanoMapper project is reaching its end, the tools and solutions it provides are maturing and are getting ready to be tested and used by researchers and practitioners in the nanosafety community.

## OBJECTIVES

The objective of the workshop was to bring together potential users of the eNanoMapper computational framework, make them familiar and train them on eNanoMapper tools and services and give them the opportunity to provide feedback and comments that will be taken into account for their final releases. The users were able to bring their own data or work based on existing examples and tutorials. The aim of the workshop was to equip the participants with the knowledge to carry out the following:

- Import data in the eNanoMapper data repository
- Annotate data with ontological terms
- Perform queries on data and visualize results
- Analyze raw experimental data such as omics data and images
- Develop, optimize and validate predictive models
- Use models for predictions
- Optimally design experiments
- Generate reports

## PROGRAM

**Exercise 1** Extracting knowledge from data using the JaqPot Modelling Tool (Philip Doganis – NTUA)

**Exercise 2** Omics Data Analysis for Nanotoxicology (Penny Nymark - MB)

**Exercise 3** Using KNIME for modelling toxicity in nanoparticles (Georgios Drakakis – NTUA)

**Exercise 4** Analyze nanotoxicity data using R (Georgia Tsiliki – NTUA)

**Exercise 5** Filling knowledge gaps in Nanotoxicology with Read Across Predictions, Practice & Requirements (Christoph Helma – IST)

## 9. EU-US nanoEHS workshop 2016, Rheinfelden, Germany, October 24-28, 2016.

Webpage: <http://nanoehs-workshop.eu/>

Organized by the eNanoMapper and BILAT, USA 4.0 projects, in connection with OpenTox Euro.



## BACKGROUND

This international event was organized in the context of the US-EU dialogue in the area of nanomaterial environmental health and safety (nanoEHS) that has as its goal to engage US and EU experts in active discussions encourage joint programs of work and to support activities of communities of research involving EU and US participation.

The theme of the workshop was “Enabling a sustainable harmonised knowledge infrastructure supporting nano environmental and health safety assessment” and the event was attended by about 30 experts.

The workshop's main objective was to facilitate networking, knowledge sharing and idea development on the requirements and implementation of a sustainable knowledge infrastructure for nanoEHS. This infrastructure should support the needs required by different stakeholders including researchers, industry, regulators, workers and consumers.

The workshop was chaired by Dr. Barry Hardy (DC). Dr Lisa Friedersdorf (National Nanotechnology Coordination Office, USA) provided the opening remarks followed by presentations and discussions under different sessions: 1. Information Needs of Stakeholders & Applications, 2. US-EU perspectives, initiatives and progress, and 3. Knowledge Infrastructure Solutions.

Presentations were given by Dr. Juan Riego Sintes (European Commission - Joint Research Centre, Italy), Peter Ritchie (Institute of Occupational Medicine, UK), Dr. John Rumble (R&R

Data Services, USA), Assoc. Prof. Stacey Harper (Oregon State University, USA), Dr. Andrea Haase (German Federal Institute for Risk Assessment), Berna Windischbaur (Austrian Research Promotion Agency), Dr. Stephanie Morris (National Institutes of Health, USA), Prof. Iseult Lynch (University of Birmingham, UK) and Dr. Barry Hardy (Douglas Connect GmbH, Switzerland). The presentations were followed by two interactive knowledge café sessions. The participants were able to use an interactive web tool (<https://summit.enanomapper.net/>), in order to access specific resources, and actively contribute to the discussions by adding new content, comments and answers related to the session topics. The presentations are also available at the above-mentioned link.

The objective of the first session on *read-across and data completeness* led by Dr. Frederick Klaessig (Pennsylvania Bio Nano Systems, USA), was to broaden awareness of data completeness while fostering best practices within the US-EU communities. The second session on *nano-ontologies* was led by Dr. Egon Willighagen (Maastricht University, The Netherlands). eNanoMapper and other initiatives have developed a substantial ontology to be used in nanotechnology and safety assessment. This ontology can be used for harmonization purposes, ensuring a common description and reporting format. Based on the case study interaction and discussions, the participants evaluated how the ontology is supporting the scientific and regulatory needs, what the gaps are and further actions. Guided by a detailed tutorial, the participants were able to browse the eNanoMapper ontology, use the ontology in searching on <http://search.data.enanomapper.net>, and finally evaluate the appropriateness of the eNanoMapper ontology by filling an evaluation survey.

The nanoEHS workshop was followed by a roundtable discussion on the EU-US Roadmap on Nanoinformatics, led by Dr. Andrea Haase. This roadmap has been jointly developed in cooperation among US, European and Canadian scientists working in the field of nanotechnology.

## 10. Nano Modelling Workshop, Rheinfelden, Germany, October 25, 2016.

Organized by eNanoMapper: Barry Hardy (Douglas Connect), Haralambos Sarimveis, Philip Doganis and George Drakakis, in conjunction with the NanoEHS workshop and OpenTox Euro 2016.

Web: <https://www.enanomapper.net/events/nano-modelling-workshop>

### BACKGROUND

Computational modelling and software tools are increasingly important to support experimental testing and risk assessment in modern nanotoxicology. The EU has given

particular emphasis to funding research relative to the development of computational methods for toxicological risk assessment of engineered nanoparticles. In particular, six modelling projects (NanoPuzzles, ModENPTox, PreNanoTox, MembraneNanoPart, MODERN, and eNanoMapper) have been funded under the FP-7 and the MODENA COST action was launched. A joint conference was organized by these projects in Malaga, Spain in September 2015 (CompNanoTox <http://compnanotox2015.eu>) and brought together researchers involved in all of these modelling projects and the MODENA COST action in order to integrate and disseminate their work and discuss further needs and perspectives in the area of computational nanotoxicology (see **Deliverable D6.2**).

The field of computational modelling in nanotoxicology is evolving, as more researchers and practitioners are starting to use and apply it, the generation of data is expanding and more emphasis is given to the interaction of nanoparticles with biological systems to investigate and understand mechanisms of actions. Building on this, the Nano Modelling Workshop objectives were:

#### OBJECTIVES

1. Give the opportunity to research groups working on computational nanotoxicology to disseminate their modelling tools based on hands-on examples and exercises
2. Present a collection of modelling tools that can span the entire lifecycle of nanotox research, starting from the design of experiments until use of models for risk assessment in biological and environmental systems.
3. Engage the workshop participants in using different modelling tools and motivate them to contribute and share their knowledge.

The workshop provided a demonstration of two applications developed within the eNanoMapper project:

- Philip Doganis (NTUA). [EXTRACTING KNOWLEDGE FROM DATA USING THE JAQPOT MODELLING TOOL](#).
- Christoph Helma (IST). [NANOMATERIAL READ ACROSS PREDICTIONS WITH NANO-LAZAR](#).

The participants had the possibility to use and test the tools, and also to discuss and give feedback to the developers.

The first demonstration offered hands-on work on the development of nanoQSAR models based on data available from the eNanoMapper database (<https://data.enanomapper.net/>),

making use of the eNanoMapper computational infrastructure from the National Technical University of Athens that extends the OpenTox API. The second demonstration included a presentation of the lazar read across framework, the adjustments of the application for nanoparticles, data requirements, comparison of algorithms and descriptors and exercises on gold and silver nanoparticles.

## 11. OPENTOX EURO 2016, Rheinfelden, Germany, October 26-28, 2016.

The OpenTox Conference included a nanosafety related session and parallel workshops, offering an excellent opportunity for various projects, including eNanoMapper, to present their results and solutions.

eNanoMapper members presented their achievements in different sessions of [OpenTox EURO 2016](#):

### Session 1: Computational Modelling of Mechanisms at the Nano Scale (Chair: Barry Hardy)

- [Predictive Modelling of Biological Effects of Engineered Nanomaterials](#) (Georgios Drakakis, NTUA)
- [Nanomaterials Design and Safety Assessment](#) (Barry Hardy, DC)

### Session 2: Translational Bioinformatics applied to Safety Assessment (Chair: Roland Grafstrom)

- [Standardization of bioinformatics analysis workflows for omics-based safety assessment](#) (Pekka Kohonen, MB)

### Session 5: Open Science Applications (Chair: Thomas Exner)

- [Open source software in Toxicology: Modeling Perspectives](#) (Philip Doganis, NTUA)

### Session 6: AOPs and Protocol Ontologies (Chair: Clemens Wittwehr)

- [Why Do We Need Ontologies?](#) (Thomas Exner, DC)

### Session 7: Emerging Methods and Practice (Chair: Ola Spjuth)

- [Data integration with identifiers and ontologies](#) (Egon Willighagen, UM)

## 12. SaferNanoDesign, Summer School at ESI, Archamps, France, June 13-18 2016.

### Background

[SaferNanoDesign](#) is a one-week intensive course on nanomaterials production, life cycle, environmental and toxicological aspects, etc. jointly organised by Université de Grenoble Alpes and Aix-Marseille Université and held at the ESI (European Scientific Institute, Archamps) within the frame of their BioHealthComputing programme. SaferNanoDesign aimed to familiarize early-stage researchers and postgraduate students (2nd year Master/PhD) with risk evaluation using computational methods of modeling and simulation relevant to nanomaterials. eNanoMapper contributed with lectures and practical sessions about biological pathway analysis using nanomaterial data and use of nanomaterial databases (eNanoMapper) for information acquisition.

**Lectures:**

- F. Ehrhart (UM) Gene expression data analysis
- F. Ehrhart (UM) Biologic networks and pathway analysis

**Practical sessions:**

- F. Ehrhart (UM) Gene expression data analysis
- F. Ehrhart (UM) Pathway and gene ontology analysis

### 13. New Tools and Approaches for Nanomaterial Safety Assessment, Final Conference, Málaga, Spain, February 7-9, 2017.

The conference is jointly organized by five FP7 projects – NANOSOLUTIONS, SUN, NANOMILE, GUIDENANO, and eNanoMapper – and aims at presenting the main results achieved in the course of the projects fostering a discussion about their impact in the nanosafety field and possibilities for future research programmes. The conference is targeted at consortium partners from the organizing projects, as well as representatives from other EU projects, industry, government, civil society and media. The eNanoMapper project will give several oral and poster presentations, and the project will also organise a “**Hackathon on templates for data collection**”, on 7 February. The hands-on exercises at this event will include demonstrations on various data management functionalities, data preparation and upload, as well as an ontology mapping exercise.

**Conference presentations:**

- The keynote presentation on behalf of the project will be given by Barry Hardy (DC), Egon Willighagen (UM), Nina Jeliaskova (IDEA), and Haralambos Sarimveis (NTUA):

## “Advancing a Sustainable Knowledge Infrastructure for the Safety Assessment of Nanotechnology”.

Additionally, several eNanoMapper members will give **oral presentations** at the meeting, along with several poster presentations describing various tools and resources developed in the project. The speakers are: Nina Jeliaskova (IDEA), Christoph Helma (IST), Egon Willighagen (UM), Philip Doganis (NTUA), Penny Nymark (MB), and Pekka Kohonen (MB) and details are provided below.

### 3.3.1 Conference presentations

The project partners have also presented or will present oral talks or posters at the following meetings during the third and final year of the project (including at the joint nanosafety conference):

| Title/Topic  | Presenting Author        | Meeting  |
|--|--------------------------|--|
| Modelling toxicity of nanoparticles using KNIME  | Georgios Drakakis (NTUA) | 2 <sup>nd</sup> Sustainable Nanotechnology Training School, Venice, Italy, January 25-29, 2016 |
| Ontology for physicochemical measurement techniques and guidelines for experimental design     | Barry Hardy (DC)         | NanoDefine NSC Synergy workshop, Neth-ER, 2 February 2016, Brussels                            |
| Bioinformatics analysis of nano-based omics data (presentation and hands-on session)           | Penny Nymark (MB)        | Hands-on workshop on Nano Safety Assessment, Basel, Switzerland, February 10, 2016             |
| eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment | Barry Hardy (DC)         | Lecture, Birmingham, UK, 23 February 2016  |
| eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment | Roland Grafström (MB)    | caLIBRAte kick-off, Helsingør, Denmark, May 18, 2016   |
| eNanoMapper - A Database and   | Penny Nymark (MB)        | Stockholm University,  |

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|---|--|--|
| Ontology Framework for Nanomaterials Design and Safety Assessment   |  | SmartNanoTox partners, 25th May, 2016  |
| Support tools for the US-EU NanoEHS scrimmage on nanomaterials spill scenario (poster)  | Barry Hardy (DC)   | International Nanotoxicology Congress 2016, Boston, USA, June 1 – 4, 2016  |
| Entering the era of Big Data: Defining and Modelling Adverse Outcomes by Omics Driven Informatics   | Roland Grafström (MB)  | University of Pamplona, Pamplona, Spain<br>7th June, 2016  |
| eNanoMapper: data management solutions  | Nina Jeliaskova (IDEA)                                       | 7th Consortium Meeting of the NANoREG project, June 8-9, 2016 in Bilbao, Spain   |
| Usefulness of HTS and Toxicogenomics space modelling to assessing NM safety   | Roland Grafström and Pekka Kohonen (MB)                      | NANoREG General Assembly and 7th Consortium Meeting, Bilbao<br>9th June, 2016  |
| eNanoMapper - a database and ontology framework for design and safety assessment of nanomaterials   | Gözde Kilic (KI) (and see published abstract, section 3.7.1) | 52 <sup>nd</sup> European Congress of the European Societies of Toxicology, EUROTOX, September 4-7, 2016, Seville, Spain |
| Nanoinformatics and data resource sustainability  | Barry Hardy (DC)   | NSC meeting 14 September 2016, Stockholm   |
| Multi-readout in vitro high-throughput screening analyses serve efficiently for evaluation and ranking of nanomaterial toxicity under diverse testing protocols (oral presentation) | Vesa Hongisto (MB)   | Nanosafety Forum for Young Scientists, Visby, Sweden, September 15-16, 2016  |
| Predictive Toxicogenomics Space (PTGS) – an omics-based tool for predictive toxicity testing (poster presentation)  | Pekka Kohonen (MB)   | Nanosafety Forum for Young Scientists, Visby, Sweden, September 15-16, 2016  |
| Applying “Big Data” for handling nanomaterials read across and adverse outcome studies (oral presentation)  | Penny Nymark (MB)  | Nanosafety Forum for Young Scientists, Visby, Sweden, September 15-16, 2016  |
| Bioinformatics analysis of nano-based omics data (presentation)   | Penny Nymark (MB)  | Hands-on workshop, Athens, Greece, September 29, 2016  |

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| and hands-on session)   |                          |   |
| NANoREG data logging: how to access NANoREG and other data  | Nina Jeliaskova (IDEA)   | Final NANoREG National Advisors and the National Coordinators meeting, The Hague, NL, Oct 11-12, 2016 |
| eNanoMapper applications to support the risk assessment of nanomaterials  | Lucian Farcal (DC)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| In silico capture of toxicity effects related to nanomaterials using a novel predictive toxicogenomics space tool (oral presentation) | Pekka Kohonen (MB)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| A pathway tool for applying “big data” in nanosafety – focussed read across the adverse outcomes studies (oral presentation)          | Penny Nymark (MB)        | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| eNanoMapper tutorials: guidance to the infrastructure for nanomaterial modeling (poster)  | Philip Doganis (NTUA)    | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| Using KNIME and Python to access and process eNanoMapper data (poster)  | Georgios Drakakis (NTUA) | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| eNM-Ontoviewer: interactive visualisation of SPARQL queries for eNanoMapper ontologies and data (poster)                              | Denis Gebele (IST)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| In silico toxicology services for nanoparticle risk assessment (poster)   | Christoph Helma (IST)    | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| Integration of the in silico toxicology services in the eNanoMapper infrastructure (poster)   | Christoph Helma (IST)    | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain       |
| In silico toxicology rest services (poster)   | Micha Rautenberg (IST)   | New Tools and Approaches for Nanomaterials Safety   |

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|  |                             | Assessment, February 7-9, 2017, Malaga, Spain   |
| Exploring correlation patterns on toxicity omics data (poster)   | Demetra Danae Varsou (NTUA) | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain |
| Mapping the Nanosafety cluster data  | Nina Jeliaskova (IDEA)      | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain |
| Answering Scientific Questions with linked European nanosafety data  | Egon Willighagen (UM)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain |
| Nanomaterials computations in your browser: predictions, read-across, experimental design and interlaboratory comparison using the JAQPOT modelling platform | Philip Doganis (NTUA)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain |
| Nano-Lazar: A framework for nanoparticle read across risk assessment   | Christoph Helma (IST)       | New Tools and Approaches for Nanomaterials Safety Assessment, February 7-9, 2017, Malaga, Spain |

*Additionally, Bengt Fadeel (KI) served as co-chair of the session on human health (in vitro) at the Joint Scientific Conference of ProSAFE and NANOREG, at OECD, Paris, France, Nov 29- Dec 1, 2016.*

### 3.4 COMMUNITY DEVELOPMENT

eNanoMapper has actively contributed to building an international nanosafety community. The community development effort within eNanoMapper aimed to support the development of user communities and their use of eNanoMapper resources and applications. This effort was built upon existing interactions with industry and academic groups developed by partners, e.g., within the EU NanoSafety Cluster, US-EU Communities of Research, OpenTox and ToxBank with stakeholders with interests in safety assessment and predictive toxicology, and other communities with interests in collaborative innovation in scientific and technology areas related to nanomaterials. The community development efforts were supported by the web site, social networking tools, interactions through virtual seminars and face-to-face workshops, and conference activities. eNanoMapper members are also members of the steering committee of the EU nanosafety cluster (Bengt Fadeel, Chair of WG8 on Systems Biology; Egon Willighagen, Chair of WG4 on Databases, succeeded by Nina Jeliaskova) and we chair one of the US-EU Communities of Research (Barry Hardy, Co-Chair of Databases and Computational Modeling for nanoEHS). Various meetings of other projects were attended, including the ProSafe meeting in Dessau (Egon Willighagen, Nina Jeliaskova) and the OECD/ProSafe meeting in Paris (Egon Willighagen, Nina Jeliaskova).

On Twitter a community was created around the @enanomapper account, following 160 accounts and followed by more than 180 other accounts (in comparison, the NSC account has about 1500 followers). Over the period of the project we send out more than 600 tweets informing our online community about new product releases, tutorials, upcoming webinars, and future events. This resulted each month in 3000 to 10000 tweet impressions. Our social community is mostly located in the UK (23%), USA (11%), Spain (10%), and Germany (8%).

The detailed report on community development activities in the project is provided in **Deliverable D6.4**.

### 3.5 EXPLOITATION

The exploitation seminar took place at the annual consortium meeting, in Basel, Switzerland on February 9, 2016 (workshop leader: Dario Mazzela), and included lectures, working groups and discussions. During the seminar the key exploitable resources were identified and characterized, and an elevator pitch was challenged on four selected areas (data, modelling, common language and risk assessment). The results of the elevator pitch are annexed to Deliverable 6.5. Moreover, the eNanoMapper projects has prepared a business model and exploitation plan to maintain the impact of the project after the project has finished and this is described in **Deliverable D6.5**. One of the goals of eNanoMapper was to create a collaboration

ecosystem in which partners develop specific complementary resources and competencies. Hence, in addition to individual exploitation, the capacity for collaborative exploitation through joint initiatives, tender responses and virtual organisations was explored. This capacity included technical, business, and legal elements and develop further knowledge-oriented collaborative business models. The results on user requirements and adoption developed in WP1 was considered for the exploitation strategy.

### 3.6 TUTORIALS

The applications developed within eNanoMapper are complemented by a set of support materials, dedicated to users (experimentalists, data managers, etc) or to developers. All of these dissemination and training materials were recorded, stored and made publicly available on the eNanoMapper website. During the third year of the project, a final report on the online tutorials (in total, 12) was prepared, see **Deliverable D6.3**. The tutorials aim to present step-by-step the use of specific tools and provide detailed information on the tools functionalities. The tutorials are mainly represented by electronic documents (e.g., in pdf format) or as videos. The information included in the tutorials is also a result of the developer-user interactions and represent a guideline based also on the experience accumulated during the development, testing and deployment phases. However, apart from these documents, each application has specific guidance and support materials available (additional resources, help sections, etc). The tutorials developed in the project is accessible *via* the following link: <http://www.enanomapper.net/enm-tutorials> and GitHub repository <https://github.com/enanomapper/tutorials>, and see following table:

| Title/Topic  | Author(s)  | Online resources  |
|--|--|---|
| Modelling Services: Create Dataset, Train a Model, Make a Prediction, Validate (Split, Cross or External) - Video Tutorial | Georgios Drakakis, Philip Doganis, Georgia Tsiliki, Hamos Chomenidis, Evangelia Anagnostopoulou, Haralambos Sarimveis, The National Technical University of Athens | <a href="http://www.enanomapper.net/library/modelling-services">http://www.enanomapper.net/library/modelling-services</a> |
| Jaqpot Quattro User Interface Tutorial<br>Modelling infrastructure   | Georgios Drakakis, C. Chomenidis, G. Tsiliki, E. Anagnostopoulou, P. Doganis, H. Sarimveis, The National Technical University of Athens                            | <a href="http://www.enanomapper.net/library/jaqpot-quattro-ui">http://www.enanomapper.net/library/jaqpot-quattro-ui</a>   |

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|--|--|---|
| Entering and Analysing Nano Safety Data  | Nina Jeliaskova (Idea Consult), Egon Willighagen (Maastricht University)   | <a href="http://www.enanomapper.net/library/nano-safety-data">http://www.enanomapper.net/library/nano-safety-data</a>                 |
| How to Use Chipster for Bioinformatics Analysis of Nanomaterial-Based Omics Data   | Penny Nymark (Misvik Biology), Friederike Ehrhart and Egon Willighagen (Maastricht University), Eija Korpelainen (CSC - IT Center for Science, Finland), Pekka Kohonen and Roland Grafström (Misvik Biology) | <a href="http://www.enanomapper.net/library/chipster-tool-analysis">http://www.enanomapper.net/library/chipster-tool-analysis</a>     |
| How to use the statistics module of ArrayAnalysis.org for statistics analysis of microarray data                         | Friederike Ehrhart, Lars Eijssen, Anwasha Bohler, Linda Rieswijk, Egon Willighagen (Maastricht University), Penny Nymark (Misvik Biology)  | <a href="http://www.enanomapper.net/library/statistics-analysis">http://www.enanomapper.net/library/statistics-analysis</a>           |
| Creating biological pathways for WikiPathways using PathVisio  | Friederike Ehrhart, Martina Summer-Kutmon, Egon Willighagen, Kristina Hanspers, Alexander Pico, Linda Rieswijk (Maastricht University), Penny Nymark (Misvik Biology)  | <a href="http://www.enanomapper.net/library/how-make-pathway">http://www.enanomapper.net/library/how-make-pathway</a>                 |
| How to use the AffyQC web tool of ArrayAnalysis.org for quality control and pre-processing of Affymetrix microarray data | Friederike Ehrhart, Lars Eijssen, Anwasha Bohler, Linda Rieswijk, Egon Willighagen (Maastricht University), Penny Nymark (Misvik Biology)  | <a href="http://www.enanomapper.net/library/affyqc-web-tool">http://www.enanomapper.net/library/affyqc-web-tool</a>                   |
| How to use the Pathway module of ArrayAnalysis.org for pathway analysis of microarray data                               | Friederike Ehrhart, Lars Eijssen, Anwasha Bohler, Linda Rieswijk, Egon Willighagen (Maastricht University), Penny Nymark (Misvik Biology)  | <a href="http://www.enanomapper.net/library/pathway-analysis">http://www.enanomapper.net/library/pathway-analysis</a>                 |
| How To Use All Available Functionalities Of The Jaqpot Quattro Web Application   | Georgios Drakakis, C. Chomenidis, G. Tsiliki, E. Anagnostopoulou, P. Doganis, H. Sarimveis, The National Technical University of Athens  | <a href="http://www.enanomapper.net/library/jaqpot-quattro-api">http://www.enanomapper.net/library/jaqpot-quattro-api</a>             |
| Create and use lazar nanoparticle models   | Christoph Helma, Micha Rautenberg, Denis Gebele, in silico toxicology gmbh   | <a href="https://github.com/opentox/lazar/blob/development/README.md">https://github.com/opentox/lazar/blob/development/README.md</a> |
| How to reproduce validation results of nano-lazar paper  | Christoph Helma, Micha Rautenberg, Denis Gebele, in silico toxicology gmbh   | <a href="https://github.com/enanomapper/nano-lazar-paper">https://github.com/enanomapper/nano-lazar-paper</a>                         |
| Modelling Services:  | Georgios Drakakis, Philip Doganis,   | <a href="https://www.enanomapper.net/lib">https://www.enanomapper.net/lib</a>   |

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| <p>Experimental Design, Interlaboratory Testing, Read-Across - Video Tutorial</p>                                      | <p>Georgia Tsiliki, Hapos Chomenidis, Evangelia Anagnostopoulou, Haralambos Sarimveis, The National Technical University of Athens</p>         | <p>rary/modelling-services-p2</p>  |
| <p>Jaqpot Quattro User Interface Tutorial<br/><br/>Experimental design, Interlaboratory comparison and Read across</p> | <p>Georgios Drakakis, C. Chomenidis, G. Tsiliki, E. Anagnostopoulou, P. Doganis, H. Sarimveis, The National Technical University of Athens</p> | <p><a href="https://www.enanomapper.net/library/jaqpot-quattro-ui-p2">https://www.enanomapper.net/library/jaqpot-quattro-ui-p2</a></p> |

## **3.7 PUBLICATIONS**

### **3.7.1 Peer-reviewed original articles, reviews and book chapters**

- G. Kilic, B. Fadeel, L. Farcas, H. Sarimveis, P. Doganis, G. Drakakis, G. Tsiliki, C. Chomenidis, C. Helma, M. Rautenberg, D. Gebele, N. Jeliaskova, N. Kochev, G. Owen, J. Chang, E.L. Willighagen, F. Ehrhart, L. Rieswijk, V. Hongisto, P. Nymark, P. Kohonen, R. Grafström, B. Hardy (2016). eNanoMapper – A database and ontology framework for design and safety assessment of nanomaterials. *Toxicology Lett.*, 258, Suppl., 118-119 [abstract, EUROTOX 2016].
- K. Bhattacharya, G. Kilic, P.M. Costa, B. Fadeel. (2016). Cytotoxicity and immunotoxicity profiling of nineteen nanomaterials enables hazard ranking and grouping based on inflammatory potential. [submitted for publication] [note: funded, in part, by FP7-NANOREG].
- Samuel Lampa, Egon Willighagen, Pekka Kohonen, Ali King, Roland Grafstrom and Ola Spjuth. RDFIO: Extending Semantic MediaWiki to support interoperable biological and chemical data management [submitted for publication].
- Grafström RC, Nymark P, Hongisto V, Spjuth O, Ceder R, Willighagen E, Hardy B, Kaski S, Kohonen P. Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of 'Omics' Data from Human Cell Cultures. *Altern Lab Anim.* 2015 Nov;43(5):325-32.
- Jeliaskova N, Chomenidis C, Doganis P, Fadeel B, Grafström R, Hardy B, Hastings J, Hegi M, Jeliaskov V, Kochev N, Kohonen P, Munteanu CR, Sarimveis H, Smeets B, Sopasakis P, Tsiliki G, Vorgrimmler D, Willighagen E. The eNanoMapper database for nanomaterial safety information. *Beilstein J Nanotechnol.* 2015 Jul 27;6:1609-34.
- Helma C., Rautenberg M., Gebele D. nano-lazar: Read across predictions for nanoparticle toxicities with calculated and measured properties address. (2017). [submitted to *Frontiers in Pharmacology*].
- Drakakis G, Moledina S, Chomenidis C, Doganis P, Sarimveis H., Decision Trees for Continuous Data and Conditional Mutual Information as a Criterion for Splitting Instances. *Comb Chem High Throughput Screen.* 2016;19(5):423-8.

- Tsiliki G., Nymark P., Kohonen P., Grafstrom R., Sarimveis H. Enriching nanomaterials omics data: an integration technique to generate biological descriptors. [under review in Nat Nanotechnol].
- Varsou D.D., Tsiliki G., Nymark P., Kohonen P., Sarimveis H. toxFlow: a shiny application for predicting toxicity with omics and physicochemical data data. [to be submitted to PeerJ computing].
- Chomenidis C., Drakakis G., Tsiliki G., Anagnostopoulou E., Valsamis A., Doganis P., Sopasakis P., Sarimveis H. Jaqpot Quattro: A novel computational platform that offers modelling and analysis services for nanomaterials. [submitted for publication].
- J Hastings, N Jeliaskova, G Owen, G Tsiliki, CR Munteanu, C Steinbeck, and E Willighagen. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment, *Journal of Biomedical Semantics*, March 2015, 10.1186/s13326-015-0005-5.
- Tomasz Puzyn, Nina Jeliaskova, Haralambos Sarimveis, Richard L. Marchese Robinson, Vladimir Lobaskin, Robert Rallo, Andrea-N. Richarz, Agnieszka Gajewicz, Manthos G. Papadopoulos, Janna Hastings, Mark T. D. Cronin, Emilio Benfenati, Alberto Fernandez, On the validation criteria of (Q)SAR models used in nanotechnology, submitted for publication to *Food and Chemical Toxicology*. [note: joint publication of the six modelling projects].
- Pedro M. Costa, Bengt Fadeel. Emerging Systems Toxicology Approaches in Nanosafety Assessment. In: *Nanotoxicology: Experimental and Computational Perspectives*, Editors: Alok Dhawan, Diana Anderson, Rishi Shanker, Royal Society of Chemistry. (2017) (in press).
- Philip Doganis, Georgia Tsiliki, Georgios Drakakis, Charalampos Chomenidis, Penny Nymark, Pekka Kohonen, Roland Grafström, Ahmed Abdelaziz, Lucian Farcial, Thomas Exner, Barry Hardy, Haralambos Sarimveis. Computational Modelling of Biological Responses to Engineered Nanomaterials. In: *Nanotoxicology: Experimental and Computational Perspectives*, Editors: Alok Dhawan, Diana Anderson, Rishi Shanker. Royal Society of Chemistry. (2017) (in press).

*Note: it was originally foreseen in the project description that the eNanoMapper project would write or edit a book, but during the course of the project we realized that more time was needed for other forms of dissemination activities and a traditional book would not satisfy the need to quickly spread information about new developments and tools. However, we have contributed*

to a book on nanotoxicology, with a chapter on modeling and a chapter on systems biology (see above).

### 3.7.2 Other publications, proceedings, and online resources

Rautenberg, Micha, Helma, Christoph, & Gebele, Denis. (2016). qsar-report ruby gem library [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.179038>

Nikolay Kochev, & Nina Jeliaskova. (2016). nmdataparser: nmparser-1.0.1 [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.49607>

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Helma, Christoph, Denis Gebele, & Rautenberg, Micha. (2016). lazar [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.215483>

Janna Hastings; Jiakang Chang; Egon Willighagen; Friederike Ehrhart, Linda Rieswijk, (2016) Third release of eNanoMapper ontology.

Rautenberg, Micha, Gebele Denis, Helma Christoph. (2016). lazar-rest [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.187328>

Denis Gebele, Rautenberg Micha, Helma Christoph. (2017). nano-lazar [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.250818>

Denis Gebele, Rautenberg Micha, Helma Christoph. (2017). eNanoMapper ontology viewer [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.259384>

Jiakang Chang, Egon Willighagen, Friederike Ehrhart, Linda Rieswijk, Gareth Owen, Janna Hastings. (2016). eNanoMapper Ontology [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.47111>

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Roland Grafström, Penny Nymark, Micha Rautenberg, Nina Jeliaskova, Philip Doganis, Georgia Tsiliki (July, 2016) ENM DICTIONARY <http://www.enanmapper.net/library/enm-dictionary>.

Doganis P. Open source software in toxicology: Modelling perspectives [v1; not peer reviewed]. *F1000Research* 2016, 5:2815 (slide presentation) (doi: [10.7490/f1000research.1113489.1](https://doi.org/10.7490/f1000research.1113489.1)).

Tsiliki, G., Munteanu, C. R., Seoane, J. A., Fernandez-Lozano, C., Sarimveis, H., & Willighagen, E. L. (2015, December). Using the RRegrs R package for automating predictive modelling. In *MOL2NET, international conference on multidisciplinary sciences*. <http://sciforum.net/conference/MOL2NET-1/paper/3330>

Willighagen, E., Tsiliki, G., Kohonen, P., Nymark, P., Chang, J., Owen, G., Rieswijk, L., Ehrhart, F., Helma, C., Rautenberg, M., Kilic, G., Jeliaskova, N., Doganis, P., Sarimveis, H. eNanoMapper updates and its collaborations with the community #2, 2016. NanoSafety Cluster Newsletter (7), 20-25. <http://www.nanosafetycluster.eu/newsletter.html>

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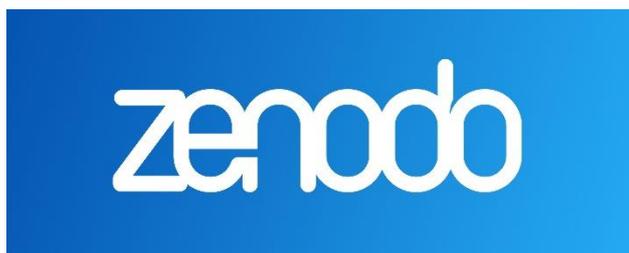
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eNanoMapper resources are accesible also via [Zenodo](#) and [OpenAIRE](#) tools.



### 3.8 FINAL ENANOMAPPER JOINT CONFERENCE



#### **New tools and approaches for nanomaterial safety assessment (Malaga, Spain)**

The final conference will be jointly organized by five FP7 projects, NANOSOLUTIONS, GUIDENANO, SUN, NANOMILE and eNanoMapper, and will take place on February 7-9, 2017 in Malaga, Spain. The aims are to present the main results achieved in the course of these projects fostering a discussion about their impact in the nanosafety field and possibilities for future research programmes. The eNanoMapper project review, and several other project meetings, will take place in conjunction with this event. The conference features 10 scientific sessions, and 5 keynote presentations, as well as a stakeholder workshop which will provide a platform for discussion that could ultimately guide the research needs that should be addressed in future projects.

Keynote speakers: Harri Alenius (FP7-NANOSOLUTIONS), Antonio Marcomini, Wendel Wohlleben, Danail Hristozov (FP7-SUN), Eva Valsami-Jones (FP7-NANOMILE), Socorro Vázquez-Campos (FP7-GUIDENANO), and Barry Hardy, Egon Willighagen, Nina Jeliaskova, Haralambos Sarimveis (eNanoMapper). With this joint conference, we hope to maximize the dissemination of our results.

For more information: [www.nmsaconference.eu](http://www.nmsaconference.eu).

## 4. CONCLUSIONS

The present report provides a summary of the dissemination and training activities during the third and final year of the eNanoMapper project. Specifically, we have highlighted our continuing efforts to provide access to different tools and resources developed in the project with tutorials on how to use these tools. We have also highlighted our role in the organization of international workshops on modelling, as well as the organization of conferences, including the 2<sup>nd</sup> Nanosafety Forum for Young Scientists (2016), an important forum for young scientists (students, post docs) across all the EU-funded nanosafety projects, and the joint nanosafety conference on "New tools and approaches for nanomaterial safety assessment" (2017), the latter event in collaboration with four other nanosafety projects funded in FP7, to mention a few events. We also organized the EU-US nanoEHS annual workshop (2016) and have been actively engaged in the EU-US nanoEHS dialogue as well as in the EU Nanosafety Cluster. As this report has shown, all the partners of the eNanoMapper project actively contributed to dissemination and training activities through webinars, scientific papers, posters and oral presentations, and tutorials. It is important to note that eNanoMapper members are actively participating in EU nanosafety cluster as well as in the US-EU nanoEHS platform. Egon Willighagen (UM) was chairing the working group on databases (on behalf of eNanoMapper) until Oct 2016, and is now succeeded now by Nina Jeliaskova (IDEA); and Bengt Fadeel (KI) is chair of the working group on systems biology (on behalf of FP7-NANOSOLUTIONS). Furthermore, Barry Hardy (DC) serves as co-chair of the community of research (or, working group) on databases and computational modeling in the US-EU joint platform on nanoEHS. We also supported the community by creating webpages for other events including the CompNanoTox conferences. The report on community development activities is provided in D6.4. Furthermore, the coordinating partner has prepared an exploitation plan to maintain the impact of the eNanoMapper project and this is described in D6.5.