



# DELIVERABLE REPORT D6.2

## eNanoMapper Year 2 Dissemination Report

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# TABLE OF CONTENTS

<b>1. EXECUTIVE SUMMARY.....</b>	<b>4</b>
<b>2. INTRODUCTION.....</b>	<b>5</b>
2.1 LIST OF DELIVERABLES.....	5
<b>3. DISSEMINATION &amp; TRAINING .....</b>	<b>6</b>
3.1 COMMUNITY WEBSITE .....	6
3.2 VIRTUAL SEMINARS.....	6
3.3 WORKSHOPS & PRESENTATIONS .....	7
3.4 COMMUNITY DEVELOPMENT .....	10
3.5 EXPLOITATION .....	11
3.6 TUTORIALS.....	11
3.7 PUBLICATIONS .....	12
3.8 FINAL ENANOMAPPER CONFERENCE.....	13
<b>4. CONCLUSION.....</b>	<b>14</b>
4.1 PLANNING FOR NEXT PERIOD .....	14
<b>5. ANNEXES.....</b>	<b>15</b>
5.1 AGENDA FOR OPENTOX 2015, DUBLIN.....	15
5.2 AGENDA FOR COMPANOTOX 2015, MALAGA.....	15
5.3 AGENDA FOR COORDINATION MEETINGS (25-26 JAN), BRUSSELS.....	15

# 1. EXECUTIVE SUMMARY

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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, and other training events. In the second year of the project, the project partners have produced additional online seminars or webinars on selected topics as well as tutorials on tools developed in other work packages and we took part in several scientific meetings with presentations on eNanoMapper, and co-organized workshops and conferences including CompNanoTox 2015 and OpenTox 2015. Important scientific papers were also published including a contribution to a thematic issue on “Nanoinformatics for Environmental Health and Biomedicine”, on the eNanoMapper database for nanomaterial safety information. Additionally, the eNanoMapper project is well represented in the EU Nanosafety Cluster as WG4 (databases) is chaired by Egon Willighagen (UM) and WG8 (systems biology) is chaired by Bengt Fadeel (KI).

## 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 will revolve around the engagement of user communities through interaction on the user requirements and use cases guiding development and through usage and evaluation of applications developed throughout the project in the other workpackages. Users will obtain 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 OpenTox and eCheminfo will be 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 will be disseminated through scientific publications and conference participations. The workshop, training and other event activities of this WP will be coordinated closely to support the community outreach activities of WP1, in addition to developing outreach to new communities and users. Based on results from WP1 and WP5 dissemination will be oriented at particular user groups, constituting different 'personas' and with different needs. Tutorials and other material developed in this WP will target the audience for which the use cases from WP5 are developed. The present report covers activities during the second year of eNanoMapper (Feb 1, 2015 to Jan 31, 2016).

### 2.1 LIST OF DELIVERABLES

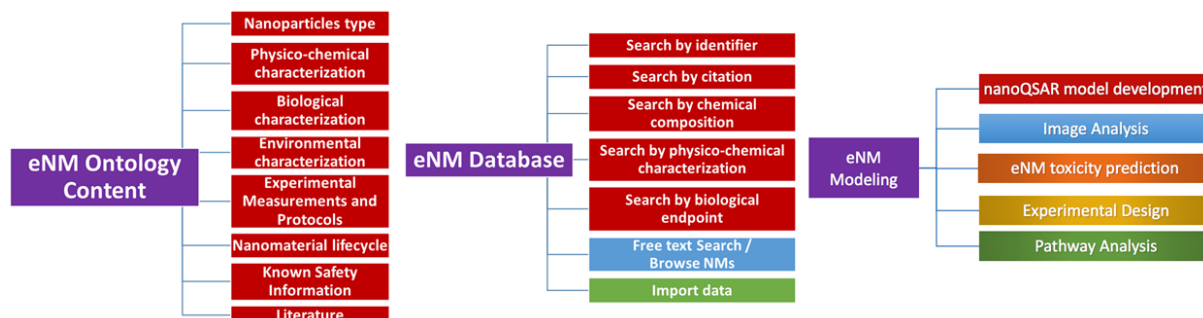
There were no deliverables during the second year, apart from the present summary report. However, in the coming year, several deliverables are due for reporting, including on community development and exploitation, as seen in the table. The community development work within eNanoMapper will focus on the development of user communities and their use of eNanoMapper resources and applications, in part through the EU nanosafety cluster and also through the US-EU nanoEHS [environmental health & safety] joint platform. This work will build on the work in WP1 on community outreach. 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. The goal will be to create a collaboration ecosystem in which a number of partners develop specific complementary resources and competencies.

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 & 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 as planned at the beginning of the project and it has been further developed (by DC) in order to build the library of webinars, tutorials, and so on (see the following sections of this report). Two new sections were created on the website in order to create a faster link to eNanoMapper released applications (<http://www.enanomapper.net/applications>) and eNanoMapper tutorials (<http://www.enanomapper.net/enm-tutorials>). The application page offers direct links to the eNanoMapper ontology page, eNanoMapper database and to various modelling tools (see schematic diagram, below). We also produced flyers to advertise the project at various events.



### 3.2 VIRTUAL SEMINARS

Virtual seminars or webinars on topics specifically related to eNanoMapper research and innovation activities, scientific applications and case studies are planned during the project and held using a virtual conferencing facility linked into the project website. To follow on the webinars held during the first year, project partners have presented the following webinars during the second year of the project, see table:

Title/Topic	Presenting Author	Date
Enriching Protein Corona Fingerprints: an Integration Technique	Georgia Tsiliki, NTUA	29th Oct, 2015
Using the eNanoMapper Ontology	Janna Hastings, EMBL-EBI	25 <sup>th</sup> June, 2015
Nanomaterial Data Visualization with Ambit.js and D3.js	Egon Willighagen, UM, and Nina Jeliaskova, IDEA	18 <sup>th</sup> May, 2015

### 3.3 WORKSHOPS & PRESENTATIONS

The eNanoMapper consortium aims to organize a series of workshops during 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. For these reasons, we aim to organize these meetings as joint events with other projects or programs. The main events during the past period were the two meetings, CompNanoTox 2015 and OpenTox 2015; see below for further details.

**HACKATHONS ON ONTOLOGY:** A working meeting was held at the EMBL-EBI in Hinxton in May 2015, with representatives from IDEA, UM and NTUA working with the EMBL-EBI team in order to efficiently evaluate the ontology for use in the different work packages and use case scenarios that the partners are involved in, most notably the use of the ontology for the organization of the database and in analysis methods. Additionally, representatives from UM, IDEA, with online participation NTUA, met in TNO in Leiden, December 2015. eNanoMapper (IDEA, NTUA) also participated in the MODENA COST Action Training School, 20-22 April 2015, in Plovdiv, Bulgaria. In addition, members of the consortium have also presented work related to eNanoMapper at several other conferences as detailed in the table below.

Title/Topic	Presenting Author	Meeting
How to Store Nanomaterial Safety Data : meet the eNanoMapper Database	Nina Jeliaskova, Nick Kochev, IDEA, Roland Grafström, MB [poster]	International Congress on Safety of Engineered Nanoparticles and Nanotechnologies SENN2015, 12-15 April 2015, Helsinki, Finland
Databases in Nanomaterial Research	Nina Jeliaskova, IDEA	MODENA COST Action Training school April 20-22, 2015, Plovdiv, Bulgaria
eNanoMapper - a Database and Ontology Framework for Nanomaterials Design and Safety Assessment	Nina Jeliaskova (IDEA), Philip Doganis (NTUA)	Stakeholders Event - FP7 Modeling projects, July 9, 2015, Thessaloniki, Greece
eNanoMapper – Enabling Systems Biology for Nanosafety	Egon Willighagen, UM	3 <sup>rd</sup> Mini-Conference on Nanotoxicology: Systems Biology in Nanosafety, Nobel Forum, KI, Stockholm, November 9-10, 2015
The eNanoMapper Infrastructure for Building Computational Toxicology Models for Engineered Nanomaterials	Haralambos Sarimveis, NTUA	CompNanoTox 2015 Meeting, Malaga, Spain, 4-6 November, 2015
eNanoMapper – a Database and Ontology Framework for Nanomaterials Design and Safety Assessment	Barry Hardy, DC	OpenTox Euro 2015 Meeting, UCD, Dublin, Ireland, 1 October 2015
The eNanoMapper Database for Nanomaterial Safety Information: Storage and Query	Nina Jeliaskova, IDEA	12th INTERNATIONAL CONFERENCE ON NANOSCIENCES &

		NANOTECHNOLOGIES (NN15) (7-10 July, Thessaloniki, Greece)
eNanoMapper – a Database and Ontology Framework for Nanomaterials Design and Safety Assessment	Barry Hardy, DC	American Chemical Society (ACS) Fall Meeting, Boston, United States, August 18, 2015
eNanoMapper - Ontology, Database and Tools for Nanomaterial Safety Evaluation	Friederike Ehrhart, UM	BBC2015, Benelux Bioinformatics Conference, Antwerp, Belgium, Dec 7-8, 2015
Using the RRegrs R Package for Automating Predictive Modelling	Georgia Tsiliki, NTUA	MOL2NET, International Conference on Multidisciplinary Science
Development of the eNanoMapper Ontology and Usability within the Nanosafety Domain	Linda Rieswijk, UM	SWAT4LS, Semantic Web Applications and Tools for Life Sciences, Cambridge, United Kingdom, December 7-10, 2015
Modelling Toxicity of Nanoparticles Using KNIME	Georgios Drakakis, NTUA	2 <sup>nd</sup> Sustainable Nanotechnology Training School, Venice, Italy, 25-29 January 2016



Figure 1: Dr. Egon Willighagen presenting at the Systems Biology meeting, Nobel Forum, 2015.

The CompNanoTox 2015 Meeting was held in Malaga (Benahavis) on 4-6 November 2015. The meeting, a joint event between eNanoMapper and several other projects in the EU nanosafety cluster, was attended by 92 persons including 2 Invited Keynote Speakers [Prof. Jerzy Leszczynski, Jackson State University, Jackson, MS; and Prof. Günter Oberdörster, University of Rochester, Rochester, NY], 39 participants from the EU COST action MODENA, 5 from the eNanoMapper Project, 5 from MembraneNanoPart, 3 from ModEnTox, 8 from MODERN, 19 from NanoPUZZLES, 3 from PreNanoTox, and 8 other participants. The



meeting was chaired by Tomasz Puzyn (NanoPUZZLES) and co-chaired by Lang Tran (COST action MODENA). In addition to the 2 keynote lectures, there were 25 platform presentations, and about 20 posters. The aim was thus to bring together the five “modeling projects” (NanoPUZZLES, ModENPTox, PreNanoTox, MembraneNanoPart, MODERN) within EU NanoSafety Cluster, along with the COST action MODENA (focused on QSAR modelling of nanomaterial toxicity) and eNanoMapper and to disseminate the results and integrate the European projects focused on developing computational methods for toxicological risk assessment of engineered nanoparticles. Prof. Haralambos Sarimveis, NTUA presented an overview of the computational infrastructure in eNanoMapper. At the meeting, discussions were initiated on a “roadmap for computational nanotoxicology”, to be developed in the frame of the EU nanosafety cluster; prof. Bengt Fadeel from eNanoMapper (and COST action MODENA) participated in the core group, which was chaired by Dr. Andrea Haase, German Federal Institute for Risk Assessment, and included Dr. Robert Rallo and Dr. Tomasz Puzyn.

eNanoMapper contribution to the event included the participation of Dr. Barry Hardy in the organization committee and as chair of one session and the building of the event-website. eNanoMapper also offered to host the CompNanoTox 2016, which has been received favourably by the conference chairs, and is progressing as a second conference to be held alongside OpenTox Euro 2016 to be held in Basel the last week in October.



Figure 2: The conference participants at the CompNanoTox meeting in Malaga, Spain, 2015.

The OPENTOX 2015 took place in Dublin, Ireland on September 30 to October 2, 2015 at the University College Dublin (UCD) and the overarching theme of the meeting was “Enabling and Strengthening Reproducible High Quality Safety Science on Complex Systems”. The meeting was co-organized by eNanoMapper and ToxBank, a data warehousing project belonging to the SEURAT-1 cluster. The meeting was co-chaired by Drs. Barry Hardy (Douglas Connect), Maurice Whelan (EC JRC), Vladimir Lobaskin (UCD), Kenneth Dawson (UCD), and Paul Jennings (Medical University of Innsbruck). The eNanoMapper project was also represented by Christoph Helma (IST) who served as working group chair for APIs (Application Programming Interfaces) for Standardization and Documentation of REST interfaces and data models of

OpenTox webservices (including eNanoMapper) on September 30. Dr. Barry Hardy presented an overview of the eNanoMapper achievements.

eNanoMapper also participated in a KNIME modelling workshop that took place at the 2<sup>nd</sup> Sustainable Nanotechnology School 2016 in (Venice; 25-29 January 2016). Data stored with eNanoMapper was used in the workshop and participants were shown how to handle file I/O, data pre-processing and modelling using several machine learning algorithms. Users were then introduced to the eNanoMapper modelling services and proceeded to use KNIME nodes to retrieve a JSON file and post it to an existing web service, thus demonstrating the potential for incorporation of eNanoMapper tools into their workflows.

Other events with eNanoMapper participation:

- EU-US Bridging NanoEHS Research Efforts workshop (12-13 March 2015, Venice, Italy)
- EU NanoSafety Cluster Meeting (15 April 2015, Helsinki, Finland)
- SUN-GuideNano Meeting (SETAC Conference) (8 May 2015, Barcelona, Spain)
- NANOTECHNOLOGY 2015 (4-11 July 2015), including 12<sup>th</sup> INTERNATIONAL CONFERENCE ON NANOSCIENCES & NANOTECHNOLOGIES (NN15) (7-10 July, Thessaloniki, Greece)
- FP7-QUALITYNANO CONFERENCE AND TRAINING WORKSHOP (15 – 17 July, Heraklion, Crete, Greece)

Additionally, eNanoMapper participated in a coordination meeting convened at DG RTD in Brussels, Belgium on January 25, 2016 focusing on data, ontology, and harmonization needs for the EU nanosafety cluster of projects, and, specifically, on the progress made by eNanoMapper in this regard. This was followed by a one-day meeting on knowledge infrastructure and framework for nanosafety. Both events chaired by Nicolas Segebarth and Georgios Katalagarianakis of the European Commission:

<http://www.enanomapper.net/events/knowledge-infrastructure-and-framework>

eNanoMapper partners also plan to participate in a workshop organized by the FP7-SUN project on February 4-5, 2016 at the Dutch Institute of Public Health and Environment, RIVM in Bilthoven. The scope of the workshop is the integration of exposure and hazard assessment in the SUN decision support system, and particularly eNanoMapper partners will assess the PROAST software and how some of its key functionalities could be integrated into the eNanoMapper web service platform.

### 3.4 COMMUNITY DEVELOPMENT

It is noted that outreach activities are covered in WP1 and its deliverables. However, in brief, the following activities and collaborations were established which also fall under community development:

- Chairing the WG4 databases (UM) and WG8 systems biology (KI) EU Nanosafety Cluster working groups and participated in meetings in Birmingham (2013), Antalya, Syracuse (2014), Helsinki, Paris (2015);
- Assumed the Chair of the EU-US Communities of Research group on Databases & Computational Modelling for NanoEHS (DC);
- Application for membership on the CEN/CENELEC TC 352 nano standards working group;
- Interacted on the ISA-Tab specification with the Oxford ISA-Tab development group;
- Interacted on the ISA-Tab-Nano specification with the US Nano WG;
- Provided advice and comments on the usage and challenges of ISA-Tab-Nano to NanoPUZZLES;
- Joined the NSC Harmonisation Initiative project group on computational modelling and engaged with this sub-cluster activity on modelling requirements and standards;

- Contributed to a common publication on nanoQSAR led by the NSC Harmonisation Initiative; Visited the EU JRC and proposed approaches to data templates and ISA-Tab for the NANoREG project. Received EU JRC Excel templates in use in NANoREG and discussed the templates in online meetings;
- Completed a data management agreement with the NANOSOLUTIONS project;
- Participated in meetings and information exchange on requirements, templates and data standards with MARINA, MODENA, SUN, GUIDENANO, NanoDefine, NANoREG, NanoPUZZLES and other NSC projects;
- Participated in meetings of and collaborating on various nanoinformatics projects with the US National Cancer Informatics Program Nanotechnology Working Group (Nano WG);
- eNanoMapper partners are actively participating in the COST action MODENA on modelling of nanomaterial toxicity (and Prof. Fadeel, KI, is a member of the Steering Committee of the action);
- Finally, we have actively worked with several cluster projects on importing data into our demonstration data warehouse and on aligning data models (database schema, templates) to the eNanoMapper ontology (NANoREG WP1 and WP6, ModNanoTox, MARINA, MODENA, NanoPUZZLES).

**The associate partner program:** <http://www.enanomapper.net/associate-partner-program>

The eNanoMapper project aims to provide standards, technologies, reference implementations and tools for the computational infrastructure of the EU NanoSafety Cluster. To ensure the alignment with the community, eNanoMapper works with a network of partners, organized in the Associate Partners Program.

### 3.5 EXPLOITATION

The exploitation seminar is scheduled for the next annual consortium meeting, in Basel, Switzerland on February 9, 2016. The exploitation workshop leader is Dario Mazzela. Moreover, the eNanoMapper projects aim to deliver a business model and exploitation plan at Month 36 (see list of deliverables above) to maintain the impact of the project after EC project funding ceases. The goal is to create a collaboration ecosystem in which a number of partners develop specific complementary resources and competencies. The results on user adoption and evaluation from WP1 will be included in the analysis.

### 3.6 TUTORIALS

The eNanoMapper project is committed to producing electronic tutorial materials which will be added to the eNanoMapper website to provide a source of self-learning material to enable users (from other projects) to understand and appreciate various eNanoMapper tools and applications:

<http://www.enanomapper.net/enm-tutorials>. The following tutorials were produced during the project period:

Title/Topic	Author(s)	Online resources
Image description Calculation Web Tool	Philip Doganis, Marios Kotsiandris, NTUA	<a href="http://www.enanomapper.net/library/image-descriptor-tutorial">http://www.enanomapper.net/library/image-descriptor-tutorial</a>
RRegrs Package Tutorial	Georgia Tsiliki, Cristian R. Munteanu, Jose A. Seoane, Carlos Fernandez-Lozano, Haralambos Sarimveis, NTUA, Egon L. Willighagen, UM	<a href="http://www.enanomapper.net/library/rregrs-package-tutorial">http://www.enanomapper.net/library/rregrs-package-tutorial</a>

Briefly, researchers at NTUA have produced an eNanoMapper tutorial on a new web tool for image analysis. Images taken by electron or fluorescence microscopy are valuable sources of information that depict the actual structure and shape of the nanomaterial. To this end, eNanoMapper has introduced a web tool which provides users with a systematic framework for the automated analysis of microscopy images of nanomaterials and the calculation of nanoparticle descriptors. This work was also presented at the recent CompNanoTox conference (see Conferences). Additionally, several eNanoMapper partners produced a tutorial on RRegrs, a collection of R regression tools based on the caret package. RRegrs 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 initial use of the tool is aimed at finding QSAR models for chemoinformatics / nanotoxicology in eNanoMapper and other EU projects. This work was published at the *Journal of Cheminformatics* and was also presented at Mol2Net, an online conference (see Publications). All tutorials are available on the website.

In addition, the eNanoMapper consortium has established a list of tutorials to be created and added successively to the eNanoMapper online library; these include tutorials targeted at each of the main topics in eNanoMapper, i.e., ontologies, databases, and analysis & modeling, as well as user application development including how to prepare and import data into the eNanoMapper database.

### 3.7 PUBLICATIONS

1. Tsiliki G, Munteanu CR, Seoane JA, Fernandez-Lozano C, Sarimveis H, and Willighagen EL. Using the RRegrs R package for automating predictive modelling, Mol2Net, 2015, 1(F), pp. 1-3, *Scientific Software*, DOI: [10.13140/RG.2.1.2050.2486](https://doi.org/10.13140/RG.2.1.2050.2486) [online conference proceedings].
2. Tsiliki G, Munteanu CR, Seoane JA, Fernandez-Lozano C, Sarimveis H, and Willighagen EL. RRegrs: an R package for computer-aided model selection with multiple regression models. *J Cheminform*. 2015, 7:46.
3. Fadeel B, Fornara A, Toprak MS, and Bhattacharya K. Keeping it real: The importance of material characterization in nanotoxicology. *Biochem Biophys Res Commun*. 2015;468(3):498-503. [included in a special issue on "Nanomedicine", guest editors: C. Alexiou, Erlangen, B. Fadeel, KI].
4. Jeliaskova N Doganis P; Fadeel B, Grafstrom R, Hastings J, Jeliaskov V, Kohonen P, Munteanu CR, Sarimveis H, Smeets B, Tsiliki G, Vorgrimmler D, and Willighagen E. The first eNanoMapper prototype: a substance database to support safe-by-design. *Proceedings of the 2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*. doi [10.1109/BIBM.2014.6999367](https://doi.org/10.1109/BIBM.2014.6999367).
5. 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, Sopsakis P, Tsiliki G, Vorgrimmler D, Willighagen E. The eNanoMapper database for nanomaterial safety information. *Beilstein J Nanotechnol*. 2015 Jul 27;6:1609-34. [included in a thematic issue on "Nanoinformatics for Environmental Health and Biomedicine", guest editors: R. Liu, Y. Cohen, UCLA].
6. Hastings J, Jeliaskova N, Owen G, Tsiliki G, Munteanu CR, Steinbeck C, Willighagen E. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *J Biomed Semantics*. 2015;6:10.

7. Grafström, R. C., 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. *Alternatives to Laboratory Animals*. 43 (5), 325-332.
8. Willighagen, E., Ehrhart, F., Rieswijk, L., Jeliaskova, N., Evelo, C., Farcas, L., Hardy, B., Sarimveis, H. eNanoMapper updates and its collaborations with the community, 2015. *NanoSafety Cluster Newsletter* (6), 14-17. [available at: <http://www.nanosafetycluster.eu/newsletter.html>].

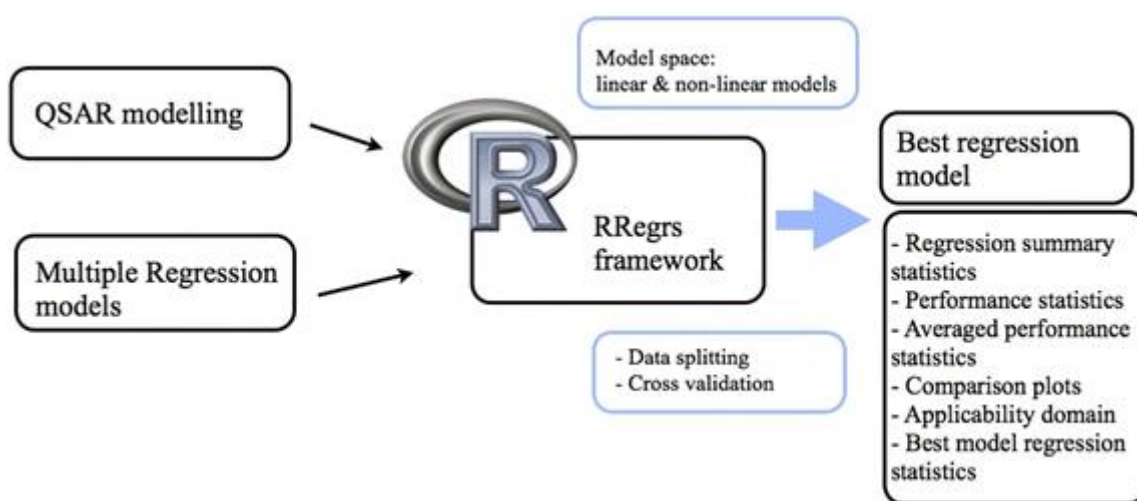


Figure 3: RRegrs: an R package for computer-aided model selection with multiple regression.

### 3.8 FINAL ENANOMAPPER CONFERENCE

The final international conference of the eNanoMapper project will focus on advanced data management, analysis and modelling topics of relevance to ENM predictive toxicology and risk assessment as implemented in the use cases of the eNanoMapper project and additionally identified situations in other research projects and industry programs, which could benefit from the integrated intelligent management of diverse data streams for risk assessment. This event will also promote eNanoMapper resources and applications to industry so as to develop partner and customer relationships and future commercial usage of the resources.

The meeting will be organised collaboratively with other relevant EU nanosafety cluster projects. The conference is currently at the planning stage and is scheduled to take place in November or December 2016, or in January 2017, to be decided at the next annual consortium meeting in Basel, February 2016.

## 4. CONCLUSION

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The present Deliverable 6.2 presents the dissemination and training activities during the second year of the eNanoMapper project. Specifically, we have highlighted our continuing efforts to provide access to different tools and resources developed in the project and instructions on how to use these tools, through online webinars, and tutorials. We have also highlighted the most recent scientific publications of the project and our involvement in the co-organization of scientific meetings and workshops, including CompNanoTox, a joint venture with several other nanosafety & modeling projects in the EU cluster.

It is also important to note that eNanoMapper partners are also actively participating in the work in the EU nanosafety cluster and in the US-EU nanoEHS alliance. Hence, Dr. Egon Willighagen (UM) is the current Chair of the working group on databases (on behalf of eNanoMapper), and prof. Bengt Fadeel (KI) is the Chair of the working group on systems biology (acting on behalf of the NANOSOLUTIONS project). Furthermore, Dr. Barry Hardy (DC), is the current EU co-Chair of the “community of research” (or, working group) on databases & computational modeling in the US-EU joint platform on nanoEHS, and participated in the annual workshop which was held in Venice, Italy in March 2015 (see annex for the agenda).

### 4.1 PLANNING FOR NEXT PERIOD

Future activities in WP6 will focus on the continued dissemination of project tools and resources, especially via the online seminars/webinars, tutorials and other training events, scientific publications and through the active participation in scientific meetings. The plans for the third and final year of the project will also take into account the discussions at the forthcoming harmonization meeting in Brussels on January 25 and 26 with the aim to identify how eNanoMapper may provide useful resources to the cluster.

We are also planning an eNanoMapper hands-on workshop on Nano Safety Assessment to be held on February 10, 2016, in Basel, Switzerland (see: <http://www.enanomapper.net/events/workshop-basel-2016>).

Other activities foreseen during the final year of the project include the organization of the 2<sup>nd</sup> Nanosafety Forum for Young Scientists, a follow-up to the first meeting which was held in Syracuse, Italy in October, 2014. The first meeting was jointly organized by the COST action MODENA and the EU nanosafety cluster while we have proposed that the second edition would be organized by eNanoMapper, with active participation and input from all the working groups in the nanosafety cluster. The meeting is scheduled for mid-September 2016 and will take place on the island of Gotland, Sweden.

Additionally, we will organize a final conference in November or December 2016 or in January 2017. We will seek to organize this event jointly with other projects in the EU nanosafety cluster. Further planning will take place at the next annual consortium meeting, scheduled to take place on February 8-10, 2016.

## 5. ANNEXES

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**5.1 AGENDA FOR OPENTOX 2015, DUBLIN**

**5.2 AGENDA FOR COMPANOTOX 2015, MALAGA**

**5.3 AGENDA FOR COORDINATION MEETINGS (25-26 JAN), BRUSSELS**

# OPENTOX EURO 2015 PROGRAM

## OPENTOX EURO 2015 CONFERENCE PROGRAM

### WEDNESDAY

#### 30 September

09.00 Short Introduction of Working Groups and Working Group Leaders:

**WG Session 1:** [APIs \(Application Programming Interfaces\)](#); WGL: [Christoph Helma \(in silico toxicology\)](#)

**WG Session 2:** [AOPs \(Adverse Outcome Pathways\)](#); WGL: [Clemens Wittwehr \(JRC\)](#)

**WG Session 3:** [Data Standards](#); WGL: [Thomas Exner \(DC\)](#)

**WG Session 4:** [Deployment](#); WGL: [Tim Dudgeon \(Informatics Matters\)](#)

10.00 Coffee Break

10.30 Working Group Sessions (*parallel tracks, coffee will be provided*):□

Joint meetings of WG1/WG4 and WG2/WG3

13.00 Lunch

14.00 Joint Working Group Session

15.00 Coffee Break

15.30 Future of OpenTox and Planning for the General Assembly Meeting ([program](#))

19.00 Social Event in Neighbourhood (*meet in Lobby of Stillorgan Park Hotel*)

### THURSDAY

#### 1 October, 2015

**Session 1: Information Requirements & Standards**, Chair: [Maurice Whelan \(EC JRC\)](#)

09.00 [Validation of Alternative Methods](#), *Maurice P. Whelan*□ □

09.25 [Validation of high throughput CALUX reporter gene assays](#), *Bart van der Burg* □

09.50 [Reliability and Relevance of Toxicogenomics](#), *Michael P. Ryan*

10.15 [Microfluidic Gene Expression](#), *Tara Dalton*□

10.40 [Reproducibility Crisis](#), *Alan W. Baird*

11.05 Coffee Break

**Session 2: Characterisation of Systems**, Chair: [Kenneth Dawson \(UCD\)](#)

11.35 [Nano-QNTR Database](#), *Hyun Yoon*□

12.00 Characterisation of Nanomaterials, *Kenneth Dawson*□

12.25 [eNanoMapper](#), *Barry Hardy*

12.50 Lunch

**Session 3: Experimental Data Generation & Processing**, Chair: [Ignacio Gonzalez Suarez \(PMI\)](#)

13.35 HCS data sharing: Overcoming the Challenges - How, What & Why, *Ignacio Gonzalez*



Suarez

□14.00 [Public Resource for Environmental Chemical High-Throughput Testing Data](#), *Keith Houck*□

14.25 [PubChem HTS data](#), *Yanli Wang*

□14.50 [ToxBank](#), *Barry Hardy*

15.15 Coffee Break

**[Session 4: Metabolism](#)**, Chair: [Carol Marchant \(Lhasa\)](#)

15.45 [Drug Metabolism Prediction](#), *Johannes Kirchmair*□

16.10 [QM P450 Predictions](#), *Matthew Segall*

16.35 [In Silico Metabolism](#), *Carol Marchant*□

17.10 Knowledge Café

□**18.15 Poster Session (sponsored by Irish Society of Toxicology) and Reception**

**FRIDAY**

**2 October, 2015**

**[Session 5: Modelling Cellular Perturbations & Responses](#)**, Chair: [Paul Jennings \(Medical Univeristy of Innsbruck\)](#)

08.45 Introduction, Paul Jennings

□09.00 [Transcriptomics Hit the Target](#), *Alice Limonciel*□

09.25 [Proteostatic-Stress in Leukemia](#), *Eva Szegezdi*□

09.50 [The Aryl Hydrocarbon Receptor](#), *Martin Leonard*□

10.15 [Omics-driven bioinformatics and modeling approaches](#), *Roland Grafström*

10.40 Coffee Break

**[Session 6: Linking Parameters & Evidence across Scales](#)**, Chair: [Vladimir Lobaskin \(UCD\)](#)

11.20 [Nanomaterial Cellular Kinetics](#), *Christoffer Aberg*□

11.45 [Nanoparticle-membrane interaction](#), *Thorsten Auth*

□12.10 [Nanomaterial Modelling](#), *Robert Rallo*□

12.35 [Limitations of Data Mining](#), *Eli Goldberg*

13.00-13.45 Lunch

**[Session 7: Knowledge Integration Supporting Decision Making](#)**, Chair: [Barry Hardy \(Douglas Connect\)](#)

13.45 [The Alternatives Conundrum](#), *John E. Doe*

□14.10 [Knowledge Integration in Modern Toxicology](#), *Michael Schwarz*□

14.35 [Evaluating systemic toxicity](#), *Gladys Ouedraogo*

15.00 [Effectopedia Knowledge Integration](#), *Hristo Aladjov*□

15.25 [Assessing Prediction Reliability](#), *Pau Carrio*

15.50 [Evidence-based Toxicology](#), *Mounir Bouhifd*

16.15 Knowledge Café Including Final Wrap Up Session

19.00 Social Event in Downtown Dublin (*meet in Lobby of Stillorgan Park Hotel*)

## Conference Programme

DAY 1 (04.11.2015)



Time	Topic	Speakers / Notes
09.00 – 10.30	MODENA workshop - results of modelling activity	Joint meeting of WG1-WG3 groups, where WG3 shows results and the remaining participants take part in the discussion
10.30 – 11.00	☐ <i>Coffee break</i>	☐
11.00 – 12.30	MODENA workshop (cont.)	
12.30 – 13.30	LUNCH BREAK	☐
13.30 – 13.50	Opening of the CompNanoTox2015 Conference	José Antonio Mena Castilla, Major of Benahavis M. Olga Guerrero-Pérez, Local Organising Committee President Tomasz Puzyn, Conference Chair Lang Tran, Conference Co-Chair
13.50 – 14.25	<b>Keynote lecture: Predictive Modelling of Nanomaterial Risk: Combining or replacing <i>in vivo</i> with <i>in vitro</i> studies?</b>	Günter Oberdörster

### SESSION 1: Bridging the experiment and modelling requirements

Chair: Gunter Oberdörster, Barry Hardy

Time	Topic	Speakers / Notes
14.25 – 14.45	Data Collection from the Nanotoxicology Literature Using ISA-TAB-Nano	Richard Liam Marchese Robinson
14.45 – 15.05	The eNanoMapper infrastructure for building computational toxicology models for engineered nanomaterials,	Haralambos Sarimveis
15.05 – 15.35	☐ <i>Coffee break</i>	☐
15.35 – 15.55	Living Cellular Sensors to Monitor Nanotoxicity Using Synthetic Biology	Urartu Ozgur Safak Seker
15.55 – 16.15	New insights on engineering applications, environmental assessment and characterization of CNTs	Dimitrios Dragatogiannis
16.15 – 17.15	POSTER SESSION	☐
18:00	End of Day 1	

DAY 2 (05.11.2015)



DAY 3 (06.11.2015)



## **Data, Ontology and Harmonisation Needs for Nano Safety Cluster & Projects**

25 January 2016

DG RTD, COVENT GARDEN, Place Charles Rogier 16, 1210 Brussels

Meeting Room 5.183

### ***Draft Agenda 1.3***

**09.30 Introduction and Objectives**, Nicolas Segebarth and Georgios Katalagarianakis (European Commission)

**09.45 eNanoMapper Resources & Interactions**, Barry Hardy (Douglas Connect)

- Current Situation: deliverables, prototypes, standards, project interactions
- Stakeholder Needs & Differences: Research, Regulatory, Industry, Civil society
- Open Discussion

**10.15 Harmonisation**

- Current Situation: available ontology and templates, interoperability: Egon Willighagen (University of Maastricht) – 20 min
- Open Discussion:
  - Subject Needs: Characterisation, Hazard, Release, Exposure, Risk assessment and management;
  - Research Needs; Regulatory Needs
  - Collaboration Opportunities and Tasks
  - Agreement on Actions

**11.15 Coffee Break**

**11.30 Data**

- Current Situation: available data management and search solutions: Nina Jeliazkova (Ideaconsult) – 20 mins
- Open Discussion:
  - Subject Needs: Characterisation, Hazard, Release, Exposure, Risk assessment and management
  - Research Needs; Regulatory Needs
  - Collaboration Opportunities and Tasks
  - Agreement on Actions

**12.30 Lunch**

**13.15 Applications and Project Needs**, Roland Grafstrom (Karolinska Institute) and Iseult Lynch (University of Birmingham)

- Current Situation: available solutions, use cases, project interactions – 20 min
- Open Discussion:
  - Collaboration Opportunities and Tasks
  - Agreement on Actions

**14.30 Cluster Needs, Impact and Sustainability,** Barry Hardy (Douglas Connect) and Peter Ritchie (IOM)

- Data Management Guidance
- Data Sharing Charter
- Harmonisation Initiative
- Sustainability Plan
- Agreement on Actions

**16.00 Conclusions**

Nicolas Segebarth and Georgios Katalagianakis (European Commission)

***16:30 End of Meeting***

# Knowledge Infrastructure and Framework for Nano Safety

26 January 2016

DG RTD, COVENT GARDEN, Place Charles Rogier, 1210 Brussels

(Remote participation by TeleConferencing and Web Conferencing also Supported)

## *Draft Agenda 1.2*

### **Objectives:**

- a) Form an integrated perspective for a Nano Safety Knowledge Infrastructure (NSKI) supporting the work activities of all stakeholders involved in the research, assessment and regulation of the safety of nanotechnology;
- b) Define the critical components of such an NSKI: stakeholders, expertise, frameworks, roadmaps, methods, resources, models, databases;
- c) Agree a guidance on how a common harmonisation approach to the NSKI, including working consensus on open standards and ontology, could be best advanced;
- d) Formulate a plan for refining the KI both for NSC needs and for supporting international engagement, refinement and collaboration (including re-use and co-working of components required by other communities) and EU-US cooperation and CoPs.

**09.00 Introduction and Objectives**, Nicolas Segebarth and Georgios Katalagarianakis (European Commission)

### **09.15 Perspectives on Resources contributing to a Knowledge Infrastructure**

09.15 Presentation of the Results of the Workshop “Data, Ontology and Harmonisation Needs for Nano Safety Cluster & Projects” (held at the EC DG RTD, Brussels 25 Jan)” eNanoMapper Coordinator, Barry Hardy (Douglas Connect)

09.30 Future Nano Needs, CODATA, John Rumble (CODATA)

09.45 References & Quality Goals, Eva Valsami-Jones (Univ. Birmingham)

10.00 Ecotoxicology, Teresa Fernandes (Heriot Watt University)

10.15 Characterisation, Keld Jensen (National Research Centre for the Working Environment)

10.30 NSC Coordination Framework, Kai Savolainen (FIOH)

### **10.45 Coffee Break**

### **11.00 Perspectives on Stakeholder Needs from a Knowledge Infrastructure**

11.00 Integrating Data and Modelling, Haralambos Sarimveis (NTUA)

11.15 Ontology and ISATab-Nano, Robert Rallo (NTUA)

11.30 QSAR Modelling, Tomasz Puzyn (University of Gdańsk)

11.45 Multi Scale Modelling Challenges, Vladimir Lobaskin (UCD)

12.00 Data Templates, Building on Learning, Peter Ritchie (IOM)

12.15 Open Discussion

**12.30 Lunch**

**13.30 Defining the Knowledge Infrastructure - Discussion**

- Knowledge Infrastructure Definition & Elaboration
- Harmonization & Standards Components
- Data Management & Sharing Guidance
- Communications & Engagement
- Sustainability Plan
- Operationalising

**14.30 International Perspective – US initiatives and Cooperation with EU**

Nano WG, EU-US Scrimmage, Christine Hendren (Duke)

NNCO Nanotechnology Knowledge Infrastructure, Stacey Standridge (NNCO)

Industry & Practical Perspective, Fred Klaessig (EU-US CoP on Data and Modelling)

**15.00 Open Discussion**

**15.15 Conclusions & Actions**

eNanoMapper Coordinator, Barry Hardy (Douglas Connect)

***15:30 End of Meeting***