



# DELIVERABLE REPORT D6.3

## D6.3 eNanoMapper Tutorials

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# 1. EXECUTIVE SUMMARY

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The applications developed within eNanoMapper are complemented by a set of support materials, dedicated to users (experimentalists, data managers, etc.) and developers. Various tools were used to document the development and testing phase (described in previous reports on specific applications), while the guidance materials dedicated to users were incorporated in presentations at different face-to-face meetings, workshops, trainings, online seminars and other similar dissemination activities which facilitated the interactions and information exchanges between eNanoMapper developers and the scientific community, the main target of these applications (*see details described in Deliverables 6.1, 6.2 and 1.4*).

All these dissemination and training materials were recorded, stored and made publicly available on the eNanoMapper website.

Further, a list of terms used within the project was prepared and made publicly available, with the same aim to help the users in understanding and implementing specific elements related to ontology, data management, modelling and risk assessment. The dictionary is accessible at: <http://www.enanomapper.net/library/enm-dictionary>

The tutorials represent another category of dissemination materials, aiming to present, step by step, the use of specific tools and provide detailed information on the tools' functionalities. The eNM series of tutorials are mainly represented by electronic documents (e.g. in pdf format) or video materials. 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 collection of tutorials developed within the project is accessible at:

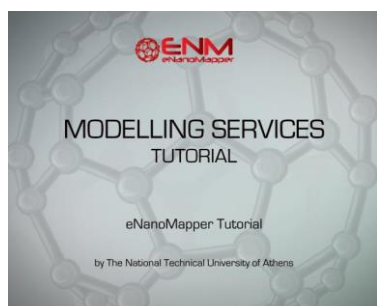
<http://www.enanomapper.net/enm-tutorials>

The tutorials are developed alongside with the applications, therefore they might also be updated once a new version or a new functionality of the application is released. For the purpose of accessibility to different raw materials used to build the tutorials (text files, Word files, etc.), we have created a repository at: <https://github.com/enanomapper/tutorials>. This will facilitate the long term and open access to different versions of the tutorials after the end of the project, and will support further developments.

All eNanoMapper tutorials are distributed under the [license CC-BY 4.0](https://creativecommons.org/licenses/by/4.0/).

## 2. LIST OF TUTORIALS

### 2.1. MODELLING SERVICES



#### CREATE DATASET, TRAIN A MODEL, MAKE A PREDICTION, VALIDATE (SPLIT, CROSS OR EXTERNAL)

<http://www.enanomapper.net/library/modelling-services>

- JaqPot Quattro is a web application for computational modelling of nanomaterials and is being developed in the context of the eNanoMapper FP7 funded project.
- This [video](#) tutorial is about the first release of the application which includes generation of datasets, creation and validation of predictive nanoQSAR models and use of models for calculating

predictions.

**Authors:** Georgios Drakakis, Philip Doganis, Georgia Tsiliki, Charalampos Chomenidis, Evangelia Anagnostopoulou, Haralambos Sarimveis (The National Technical University of Athens)

### 2.2. JAQPOT QUATTRO UI



#### HOW TO USE THE JAQPOT QUATTRO USER INTERFACE TO CREATE AND VALIDATE NANOQSAR MODELS

<http://www.enanomapper.net/library/jaqpot-quattro-ui>

- Tutorial for the User Interface (UI) made available by the Jaqpot Quattro (JQ) modelling infrastructure.
- The resource has been made available at <http://www.jaqpot.org/>.

• At this location, users may create datasets containing nanoparticles and properties, apply PMML transformations, create and validate predictive NanoQSAR models and use the models for making predictions. Several other functionalities (optimal experimental design, interlaboratory testing, read across methods) will be available in the next release of the UI.

**Tutorial license:** CC-BY 4.0

**Authors:** Georgios Drakakis, Charalampos Chomenidis, Georgia Tsiliki, Evangelia Anagnostopoulou, Philip Doganis, Haralambos Sarimveis (The National Technical University of Athens)

## 2.3. JAQPOT QUATTRO API



### HOW TO USE ALL AVAILABLE FUNCTIONALITIES OF THE JAQPOT QUATTRO WEB APPLICATION

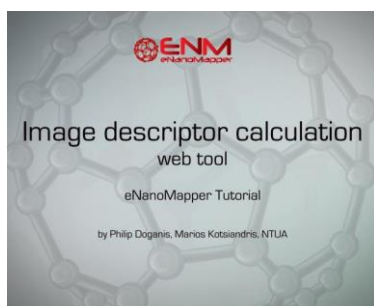
<http://www.enanomapper.net/library/jaqpot-quattro-api>

- Tutorial for the application program interfaces (APIs) available in the Jaqpot Quattro modelling infrastructure.
- The list of functionalities has been made available via the API documentation framework Swagger at <http://test.jaqpot.org:8080/jaqpot/swagger/>
- At this location, users may create datasets containing nanoparticles and properties, apply PMML transformations, create machine learning models and several other functionalities described in detail later in this document.

**Tutorial license:** CC-BY 4.0

**Authors:** Georgios Drakakis, Charalampos Chomenidis, Georgia Tsiliki, Evangelia Anagnostopoulou, Philip Doganis, Haralambos Sarimveis (The National Technical University of Athens)

## 2.4. IMAGE DESCRIPTOR TUTORIAL



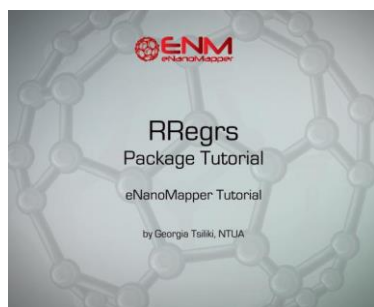
### IMAGE DESCRIPTOR CALCULATION WEB TOOL

<http://www.enanomapper.net/library/image-descriptor-tutorial>

- The 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, we introduce a web tool, which provides the user with a systematic framework for the automated analysis of microscopy images of nanomaterials and the calculation of nanoparticle descriptors.
- The term Descriptors or factors has been adopted to refer to significant properties of nanoparticles, as they describe not only the morphology of the nanoparticle but also its behavior.
- The scope of this tutorial lies mainly in providing a guide to members of the nanotoxicology community that wish to derive nanomaterial descriptors from microscopy images of nanomaterials using the image descriptor calculation web tool presented here.

**Authors:** Philip Doganis, Marios Kotsiandris (The National Technical University of Athens)

## 2.5. RREGRS PACKAGE TUTORIAL



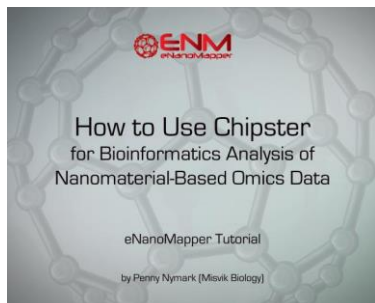
### RREGRS: PACKAGE TUTORIAL

<http://www.enanomapper.net/library/rregrs-package-tutorial>

RRegs is a collection of R regression tools based on the caret package. It is used to find the best regression models for any numerical dataset. The initial use of the script is aimed at finding QSAR models for chemoinformatics / nanotoxicology for eNanoMapper European project.

**Authors:** Georgia Tsiliki (NTUA), Cristian R. Munteanu (Maastricht University), Jose A. Seoane, Carlos Fernandez-Lozano, Haralambos Sarimveis (NTUA), Egon L. Willighagen (UM)

## 2.6. CHIPSTER TOOL FOR ANALYSIS



### HOW TO USE CHIPSTER FOR BIOINFORMATICS ANALYSIS OF NANOMATERIAL-BASED OMICS DATA

<http://www.enanmapper.net/library/chipster-tool-analysis>

- This tutorial will get you started on the basic use of the bioinformatics tool Chipster, an alternative to ArrayAnalysis.org described in other eNM tutorials.
- It will guide you through the import of microarray data (Affymetrix .CEL files), quality checks, normalization, pre-processing, basic statistical analyses methods and visualization of your data.
- Chipster is not specific to the nanosafety field, but this tutorial will be focused on the specific needs of nanotoxicological research.
- Demo version for testing: [pre-made sessions](#) (username and password: guest) (the account does not allow running analysis)

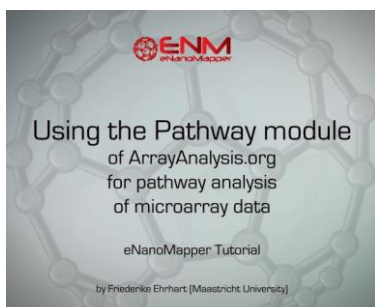
**Tutorial license:** CC-BY 4.0

**Authors:** 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)

#### External Chipster tutorials

- [YouTube](#)
- [ELIXIR Finland](#)

## 2.7. PATHWAY ANALYSIS



### HOW TO USE THE PATHWAY MODULE OF ARRAYANALYSIS.ORG FOR PATHWAY ANALYSIS OF MICROARRAY DATA

<http://www.enanmapper.net/library/pathway-analysis>

- PathVisio and ArrayAnalysis.org are open source, free to use online platforms for analysis of microarray data - and an alternative program for Chipster.
- This tutorial shows how to use the Path module (Pathway module, PathVisio webtool) of ArrayAnalysis which is designed for doing pathway analysis on microarray data.
- All source code has been written in R and is available at [https://github.com/BiGCAT-UM/Path\\_Module](https://github.com/BiGCAT-UM/Path_Module).

**Tutorial license:** CC-BY 4.0

**Authors:** Friederike Ehrhart, Lars Eijssen, Anwasha Bohler, Linda Rieswijk, Egon Willighagen (Maastricht University), Penny Nymark (Misvik Biology)

## 2.8. HOW TO MAKE A PATHWAY



### CREATING BIOLOGICAL PATHWAYS FOR WIKIPATHWAYS USING PATHVISIO

<http://www.enanmapper.net/library/how-make-pathway>

- This tutorial shows users how to make a biological (or biochemical) pathway for WikiPathways using the software PathVisio.
- The information and images are derived from help pages of WikiPathways with some recent updates.
- Pathways can be created, for example from comprehensive images, showing the interactions of genes, proteins and metabolites in

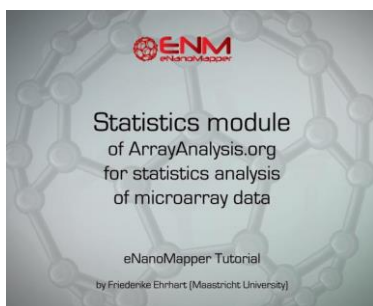
a good graphical way.

- Pathways can show molecular biological interactions like signal cascades, enzyme reactions, transport mechanisms of “healthy” pathways, drug or nanoparticle interactions, adverse outcome pathways and diseases.
- You can find examples for nanomaterial specific pathways and discussions in the nanomaterials portal of WikiPathways.

**Tutorial license:** CC-BY 4.0

**Authors:** Friederike Ehrhart, Martina Summer-Kutmon, Egon Willighagen, Kristina Hanspers, Alexander Pico, Linda Rieswijk (Maastricht University), Penny Nymark (Mlsvik Biology)

## 2.9. STATISTICS ANALYSIS



### HOW TO USE THE STATISTICS MODULE OF ARRAYANALYSIS.ORG FOR STATISTICS ANALYSIS OF MICROARRAY DATA

<http://www.enanmapper.net/library/statistics-analysis>

- ArrayAnalysis.org is an open source, free to use online platform for analysis of microarray data - and an alternative program for Chipster.
- This tutorial shows how to use the statistics module of ArrayAnalysis which is designed for doing statistics on pre-processed (quality controlled, normalized data - e.g. from the previous step using AffyQC module) microarray data.

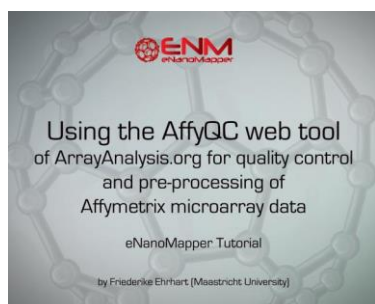
- All source code has been written in R and is available at [https://github.com/BiGCAT-UM/Stat\\_Module](https://github.com/BiGCAT-UM/Stat_Module)

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**Authors:** Friederike Ehrhart, Lars Eijssen, Anwasha Bohler, Linda Rieswijk, Egon Willighagen (Maastricht University), Penny Nymark (Karolinska Institutet)



## 2.10. AFFYQC WEB TOOL



### HOW TO USE THE AFFYQC WEB TOOL OF ARRAYANALYSIS.ORG FOR QUALITY CONTROL AND PRE-PROCESSING OF AFFYMETRIX MICROARRAY DATA

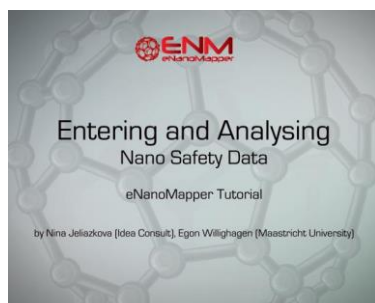
<http://www.enanomapper.net/library/affyqc-web-tool>

- ArrayAnalysis.org is an open source, free to use online platform for analysis of microarray data - and an alternative program for Chipster.
- ArrayAnalysis is a webtool, so there is no need to download it or for an access code, and it provides more extensive quality control than Chipster but it is limited to two microarray formats: Affymetrix and Illumina.
- The exact microarray type (e.g. Affy-1) is automatically recognised.
- This tutorial shows how to use the Affymetrix quality control (affyQC) module which is designed for doing quality control and preprocessing of microarray data from Affymetrix microchips.
- All source code has been written in R and is open-source, available under the Apache License version 2.0.

**Tutorial license:** CC-BY 4.0

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## 2.11. NANO SAFETY DATA



### ENTERING AND ANALYSING NANO SAFETY DATA

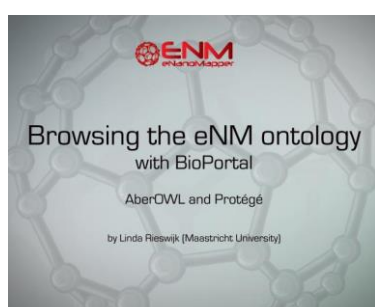
<http://www.enanomapper.net/library/nano-safety-data>

- The goal is to make the users familiar with the eNanoMapper solutions for data management and data access.
- This tutorial shows how the <http://data.enanomapper.net/> integrates various data sets, how you can search for materials, how you can upload data, and how the application programming interface (API) can be used to access data.

**Tutorial license:** CC-BY 4.0

**Authors:** Nina Jeliaskova (Idea Consult), Egon Willighagen (Maastricht University)

## 2.12. BROWSING THE ONTOLOGY



### BROWSING THE ENM ONTOLOGY WITH BIOPORTAL, ABEROWL AND PROTÉGÉ

<http://www.enanomapper.net/library/browsing-ontology>

- The field of engineered nanomaterials is exponentially growing as well as the demand to assure the safe use of this type of materials.
- Nanomaterials are defined as being materials with at least one external dimension in the size range from approximately 1 - 100 nm.

- Nanoparticles are objects with all three external dimensions at the nanoscale. Engineered nanomaterials can be used within a numerous amount of applications such as:
  1. In the design of pharmaceuticals specifically targeting organs or cells in the body such as cancer cells which also enhances the effectiveness of therapies;
  2. To make materials such as cloth or cement stronger and lighter;
  3. Use in electronics, as environmental remediation or clean - up to bind with and neutralize toxins, for their anti - bacterial function in cosmetics etc.

**Authors:** Linda Rieswijk, Friederike Ehrhart and Egon Willighagen (Maastricht University)