



NanoCommons

Nano-Knowledge Community



Philip Doganis, NTUA

### *Online Jaqpot Hackathon -*

***Take your research from the bench to the community by making  
your models available as a web service***

***NanoCommons Workshop, 2020-06-03, #nanocommons***

***This project has received funding from the European Union Horizon 2020  
Programma (H2020) under grant agreement no. 731032.***

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# Welcome



## Working Group A

# Communication, Training & Education

[Home](#) / [Overview](#) / [NSC Structure](#) / [Working Groups](#) / [Working Group A](#)



Martin Himly, Chair



Stella Stoycheva, Co-chair

## Overview

### Ambition of Work Group A

Working Group A (WGA) focuses on **cross-linking all currently active projects** in the NanoSafety Cluster. In addition, WGA endeavors to **align all training offers** in nanosafety projects and **beyond**, This effort shall be including the research fields of microplastics', advanced/innovative materials', or nanomedicines' safety assessment. Joint educational strategies are developed with representatives from the currently ongoing projects. The main activity to facilitate this essential and fruitful cross-talk between the people that are actively involved in the work of the projects is executed by **informative webinars and virtual training sessions**. Due to this cross-linking initiative across different projects secondments of early-stage researchers to other expert centers may be envisioned.




# Welcome

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- **Organization by**

- National Technical University of Athens (NTUA)
- The University of Birmingham (UoB)
- Biomax Informatics AG (Biomax)
- United Kingdom Center Ecology Hydrology (UKCEH)
- BioNanoNet (BNN)
- Paris Lodron University of Salzburg (PLUS)

- **Presenters and Practical supervisors**

- Philip Doganis: <orcid:0000-0002-0628-8434>; @PDoganis 
- Irini Liampa: <orcid:0000-0002-6350-6776>; @irliampa 
- Pantelis Karatzas
- Iseult Lynch: <orcid:0000-0003-4250-4584>; @iseult5 
- Dieter Maier: [dieter.maier@biomax.com](mailto:dieter.maier@biomax.com)

- **For training in NanoCommons & in NanoSafety Cluster**

- Martin Himly <orcid:0000-0001-5416-085X>  
[martin.himly@sbg.ac.at](mailto:martin.himly@sbg.ac.at)

# Agenda (in CEST)

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- 10:00 - Introduction round and background to the NanoCommons platform
- 10:10 - Preparation for the hands on session - setting up anaconda
- 10:30 - Introduction to Electronic Laboratory Notebooks (ELN)
- 10:45 - Introduction to the NanoCommons Knowledge Base (NC KB)
- 11:00 - Introduction to the Jaqpot suite of tools
- 11:20 - Virtual coffee break (incl time for Q&A)*
- 11:30 - Jaqpot hands-on session
- 11:40 - Jupyter: Setting up + brief intro to what you need to get started in python
- 11:50 - Importing and exploring the dataset
- 12:00 - Basic preprocessing
- 12:10 - Creating a local model and its evaluation
- 12:20 - Short break*
- 12:25 - Uploading your model to Jaqpot: You now have your web service! -  
Exploring your model on Jaqpot (adding information, QMRF report, Discussions)
- 12:35 - Using the model to get predictions on the web and in Python
- 12:45 - Explore the platform, create more models and give us your ideas
- 13:10 - Summary and Wrap up
- 13:15 - Virtual drinks and time for personal Q&A*

# Tell us briefly about your work

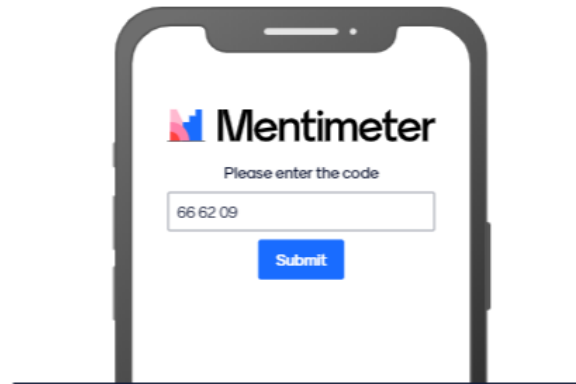
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**www.menti.com**

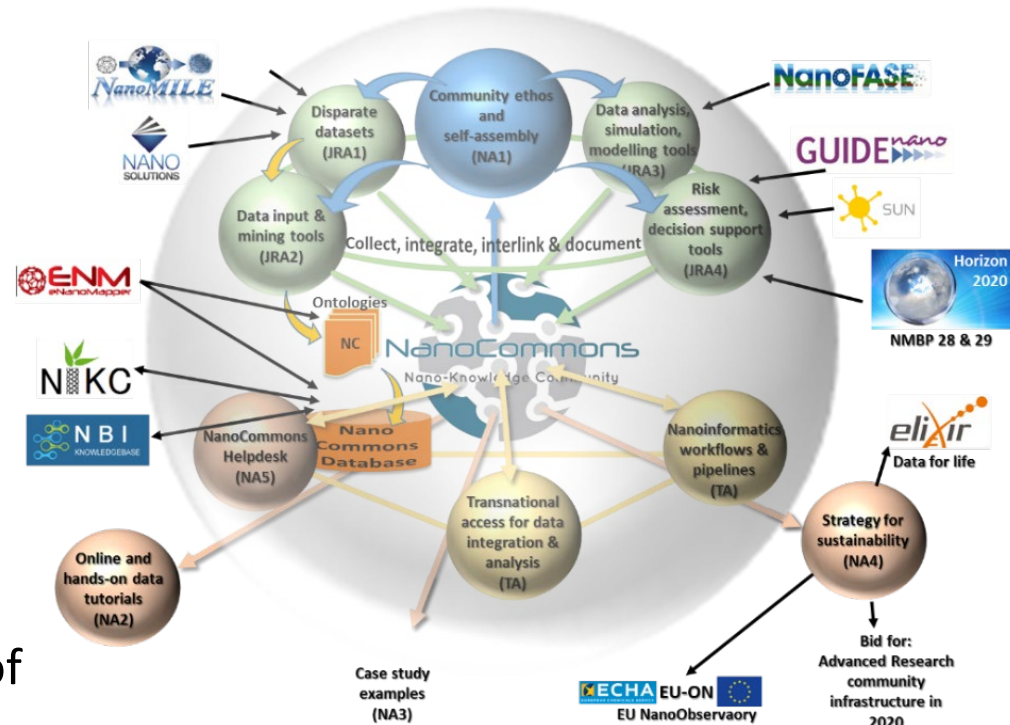


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# The idea - problem & solution

- **Nanotechnologies** are a major area of **investment & growth for the European economy**
- Knowledge and **data** remain **fragmented** and inaccessible **hampering progress**
- **Read-across approaches** are **currently absent for NMs**, but would reduce the cost and time of nanosafety research and regulation



NanoCommons is creating an **e-infrastructure** platform for reproducible science, **enhancing data integration & enabling nanoinformatics workflows** to address these gaps

# Data FAIRness

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- To remove **barriers** for nanosafety **regulatory and industry** processes
- To develop an **integrated knowledgebase** to facilitate development and application of regulatory tools such as **grouping & read-across**
- To create an **interconnected community** *via* a **FAIR data single market**
- To enable **full exploitation of EU-funded research data** & promotion of **data-driven innovation** leading to **positive socioeconomic impact**





# NanoCommons provides...

- NanoCommons **integrates the nanomaterials communities** around an agreed set of approaches for **data generation, data management and nanoinformatics** to support the risk and hazard assessment of NMs
- NanoCommons is **integrating and developing tools and services** for use by the nanomaterials communities



Experimental Workflows  
Design & Implementation



Data Processing  
& Analysis



Data Visualisation  
& Predictive Toxicity

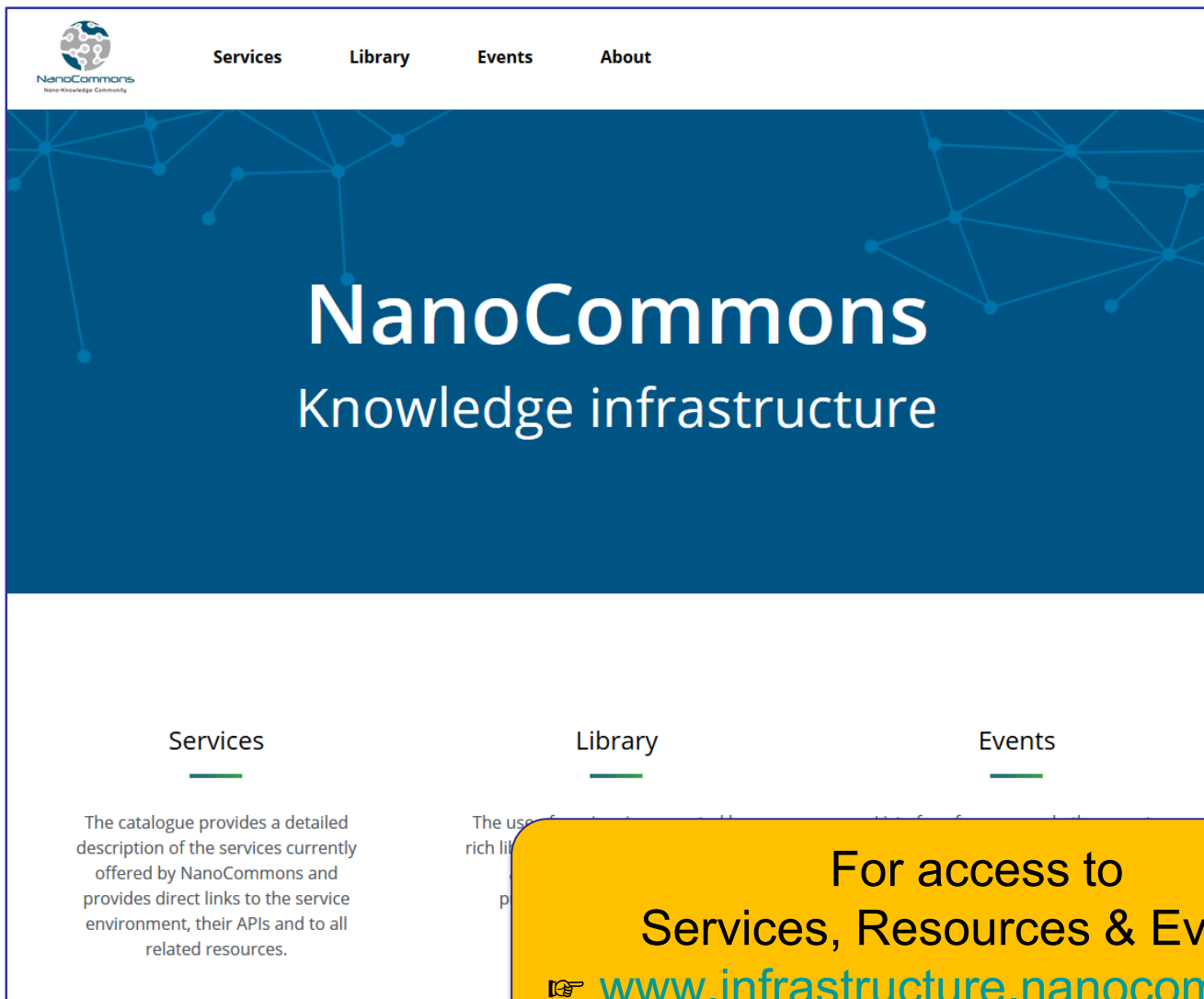


Data Storage  
& Online Accessibility

- These tools and services can be **accessed** through the **NanoCommons Transnational Access scheme**
- NanoCommons provides **Trainings**, accessible through the **NanoCommons Infrastructure Platform**: <https://infrastructure.nanocommons.eu/>



# NanoCommons Knowledge Infrastructure



The screenshot shows the NanoCommons Knowledge Infrastructure website. The header features the NanoCommons logo and navigation links for Services, Library, Events, and About. The main banner displays the title "NanoCommons Knowledge infrastructure" in white text on a blue background with a network diagram. Below the banner, there are three columns: "Services" with a description of the catalogue, "Library" with a description of the rich library, and "Events" with a description of the events. A yellow callout box at the bottom right provides access information.

NanoCommons  
Nano-Knowledge Community

Services Library Events About

## NanoCommons

Knowledge infrastructure

Services

The catalogue provides a detailed description of the services currently offered by NanoCommons and provides direct links to the service environment, their APIs and to all related resources.

Library

The use of ... with ... the ... of ...

Events

For access to  
Services, Resources & Events:  
[www.infrastructure.nanocommons.eu](http://www.infrastructure.nanocommons.eu)

## Services

The NanoCommons e-infrastructure aims to integrate and further develop existing state-of-the-art tools and to develop those that are needed to fill in the experimental, computational and beyond needs of the nanosafety community. The services are covering several areas, like data storage and online accessibility, data visualisation and predictive toxicity, data processing and analysis or experimental workflow design & implementation.

Category  Service type  Targeted users

### Jaqpot 5 Computational Platform for In Silico Modelling

Train, deploy and share predictive statistical and machine learning models

Jaqpot 5 is a user-friendly web-based e-infrastructure that allows model developers to deploy their predictive models and share them through the web. The Jaqpot 5 GUI directs the model developers ...

Provided by: National Technical University of Athens

Type: Modelling tool

Applicability domain: Hazard assessment, Risk assessment, Exposure assessment

Topic: Read-across, (Quantitative) structure-activity relationship (SAR / QSAR), Information extraction, Kinetics / biokinetics, Predictive modelling

[DETAILS →](#) [VISIT SERVICE →](#)

### Enalos Cloud Nanoinformatics Platform A Safe-by-Design Tool for Functionalised Nanomaterials

Nanoinformatics Enalos Nanomaterials Safe-by-Design

Provided by: NovaMechanics Ltd

Type: Modelling tool

Applicability domain: Hazard assessment, Risk assessment, Risk characterisation

Topic: Read-across, (Quantitative) structure-activity relationship (SAR / QSAR), Predictive modelling, Toxicology

[DETAILS →](#) [VISIT SERVICE →](#)

## Events



Services

Library

Events

About

Category



Organisations involve



Role



Filter

Reset

Submit an event

Event	Organisations involved
<b>11th World Congress on Alternatives and Animal Use in the Life Science Conference</b> 22 – 26 Aug 2021 / Maastricht, NL	Universiteit Maastricht (UM)
<b>Online Jaqpot Hackathon - Take your research from the bench to the community by making your models available as a web service</b> Webinar, Hackathon, Training, Workshop (organized by NanoCommons) 3 Jun 2020 / Online	The University of Birmingham (UoB) Edelweiss Connect GmbH (EWC) United Kingdom Research and Innovation (UKRI) National Technical University of Athens (NTUA) BioNanoNet (BIONANONET) Universitat Salzburg / Paris Lodron University of Salzburg (PLUS) BIOMAX Informatics AG (BIOMAX)
<b>EOSC-hub Week 2020</b> Conference 18 – 20 May 2020 / Online	Edelweiss Connect GmbH (EWC)
<b>Annotating Your Experimental Data workshop</b> Webinar, Hackathon, Training, Workshop (organized by NanoCommons) 28 Apr 2020 / Online	The University of Birmingham (UoB) Edelweiss Connect GmbH (EWC) United Kingdom Research and Innovation (UKRI) BioNanoNet (BIONANONET) Universitat Salzburg / Paris Lodron University of Salzburg (PLUS) Universiteit Maastricht (UM)
<b>Ontology Meeting</b> Meeting (co-organized by NanoCommons)	The University of Birmingham (UoB) Edelweiss Connect GmbH (EWC)

# NanoCommons Knowledge Infrastructure

## Library

This page contains resources and training materials to support NanoCommons users in getting familiar with the services and tools available in the infrastructure. On top of tutorials and video demonstrations, you will also find information on our publications (e.g. peer-review articles, presentations, posters) that may help you further in learning about NanoCommons concepts and implementations.

Category

Target audience

Organisations involved

Service

Submit a resource

Filter

Reset

Introduction to data /metadata management in nanosafety assessment workflows

Webinar recording

A. Papadiamantis, E. Valsami Jones, I. Lynch - University of Birmingham, UK M. Himly, University of Salzburg, AT

18 Oct 2019

↓

OpenRiskNet webinar recordings

Webinar recording

10 Sep 2019

→ OpenRiskNet library

↓

Introduction webinar to Guidenano risk assessment tool

Webinar recording

9 Sep 2019

↓

Introductory video on Nanoinformatics Model for Zeta Potential Prediction Powered by Enalos Cloud Platform

Video

9 Sep 2019

↓

# TA Calls

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- NanoCommons Transnational Access (TA) provides **funded access** to state of the art **nanoinformatics and data management tools and modelling and risk assessment services**, and the expertise to implement them successfully.
- Researchers from academia and industry are invited to access the **NanoCommons services, facilities and knowledge** to advance their work, solve problems and take their research to the next level



## Experimental Workflows Design & Implementation

*Automated data acquisition, online lab-books, data curation templates, nanoinformatics implementation*



## Data Processing & Analysis

*From data cleansing, mining and analysis to modelling*



## Data Visualization & Predictive Toxicity

*Omics, QSARs, modelling and risk assessment tools*



## Data Storage & Accessibility

*Data repositories, storage, harmonized and interoperable online access*

# How to apply for a TA...

## Transnational Access

Looking forward to working with you!

Home / Transnational Access


### Transnational access

The NanoCommons Transnational Access (TA) is the ability of nanosafety Researchers from industry, academia and regulatory bodies to access the state-of-the-art NanoCommons expertise free of charge and take advantage of the NanoCommons services, facilities and knowledge to advance their work, solve problems and take their research to the next level.

Goto the services and get in touch with the experts to design your application

# Small selection of Online Training Tools

TA service category	Nanoinformatics services	Training formats	Level
Experimental workflow	PC characterization protocols	Written tutorial	Basic
Data processing & analysis	Biomax data templates	Recorded webinar	Basic
	NIKC data templates	Written tutorial	Advanced
	Jaqpot platforms 4 & 5	Demo video	Advanced
		Demo video	Expert
	Enalos NanoXtract for TEM image analysis	Demo video	Basic
		Online tutorial	Basic
	Biocorona <i>in silico</i> modelling	Recorded webinar	Advanced
	OpenRiskNet e-infrastructure	Recorded webinars incl. demo videos	Basic
Recorded webinars incl. videos and documentations		Advanced	
Data visualization & toxicity prediction	Enalos cloud for zeta potential	Demo video	Basic
		Recorded webinar	Basic
	Enalos cloud for Safe-by-Design	Demo video	Basic
		Online tutorial	Basic
Data storage	GUIDEnano		
	SciNote		
	ACEnano Knowledge		

For access to  
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