

The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

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Summary

In the first two years of the NanoCommons project, the focus of the joint research activities workpackages (JRAs, WPs 3-6) was on making the nanoinformatics services, *i.e.* virtual tools, ready for provision as services to the nanosafety researchers via the calls for transnational access (TA). As part of this, dedicated training materials, in particular **online training resources linked directly to the NanoCommons' catalogue of services**, were also developed and are available in the NanoCommons library. Among the types of training materials developed are: (1) resources prepared for use in NanoCommons workshops and hackathons (organized to demonstrate the use and application of the selected virtual tools via dedicated training sessions with internal or external audiences); (2) self-guided tutorials, both text-based and videos; (3) suggestions for how the tools/services can be used by end-users users; and (4) case study demonstrations are being developed. Online **accessibility** of the training resources has been established via the infrastructure section of the NanoCommons project website. The **visibility** of the available online training resources has been strongly promoted, to support uptake by other ongoing EU projects working on the nanosafety topic. This was achieved through presentations at a number of highly interactive events, such as joint project or scientific meetings, industry events, and meetings involving attendees of the new member states.

This report presents the training measures implemented by NanoCommons, illustrated with concrete examples of activities in this area. A complete list of training resources (including training materials from workshops and hackathons, as well as video or written tutorials and publications) is available in the project <u>online Library</u>.



Abbreviations

- API Application Programming Interface
- EMMC European Materials Modelling Council
- EU European Union
- FAIR Findable, Accessible, Interoperable, Re-usable
- MODA Modelling Data Generalisation
- NCI National Cancer Institute
- NIKC NanoInformatics Knowledge Commons
- NP Nanoparticle
- NRG Nano-Risk Governance
- NSC NanoSafety Cluster
- NTUA National Technical University of Athens
- OWL Web Ontology Language
- Q&A Questions & Answers
- TA Transnational Access
- TRL Technology Readiness Level
- UCD University College Dublin
- URL Uniform Resource Locator
- WGF NanoSafety Cluster Working Group F on Data Management



Introduction

In this document, we report on the training activities undertaken in the first 2 years of the project and the underlying activities implemented to maximise their impact. The format of the training activities envisaged in NanoCommons includes **face-to-face meetings** (demonstration and hands-on sessions including hackathons) and **online (virtual) activities**. The latter can be live events (webinars) or recordings that allow the user to access the training resources at any convenient time (*see* **Deliverable 8.1** *for a detailed description of these type of activities*). These were designed and optimised to address the requirements and training needs of specific stakeholder groups, taking into account their level of expertise (basic, advanced, expert). As shown in **Deliverable 8.1**, the users of NanoCommons were categorised as academic researchers and students involved in fundamental or applied research nanotechnology informatics projects but also in interdisciplinary areas, researchers from industry focused on innovation and regulatory questions, regulators that need to understand the applicability and limitations of existing nanosafety risk assessment tools, and business and Health & safety managers who need to keep up to date with developments in the field in order to make informed decisions, etc.

This report presents the training measures implemented by NanoCommons with concrete examples of activities delivered to date in each type of training activity. A complete list of resources (including training materials, video or written tutorials and publications) is available in the **online Library**¹.

In order to make these activities and the resources generated by the training activities (e.g. recordings, presentations, etc.) available to NanoCommons users including those considering applying for Transnational Access (TA), an approach first developed in the e-infrastructure project OpenRiskNet² to link its services with the associated training materials and case studies, has been implemented in order to collect, describe and interlink different resources (see **Figure 1**). In this way, the users of services profit from complete and easily accessible information.



Figure 1. Representation of the NanoCommons approach to capturing and linking different resources related to the training events, NanoCommons services and related training materials.

¹ <u>https://infrastructure.nanocommons.eu/library/</u>

² <u>https://openrisknet.org/library/</u>



The NanoCommons catalogues (currently Events, Library and Services) are available at https://infrastructure.nanocommons.eu/):

- **Events** Collection and description of the events organised or attended by NanoCommons members and relevant to its stakeholders.
- Library Collection of resources and training materials to support NanoCommons users in getting familiar with the services and tools available in the infrastructure. In addition to tutorials and video demonstrations, users will also find information on our publications (e.g. peer-reviewed articles, presentations, posters) that may help them further in learning about NanoCommons concepts and implementation.
- Services Collection of NanoCommons TA services covering data storage and online accessibility, data visualisation and predictive toxicity, data processing and analysis or experimental workflow design & implementation. The training materials are directly linked to the relevant service, and as per the recommendation from the 1st periodic review, links to demonstration case studies and/or suggested user "projects" are currently being integrated.

Access to training materials relevant to NanoCommons services

The NanoCommons catalogues aim to facilitate the access of users to different training materials. The **Library**³ gathers resources and training materials (e.g. video recordings, peer-reviewed publications, posters, tutorials, presentations, reports or other public communication items) relevant to NanoCommons activities and its TA services. The Library catalogue aims to support users in finding and accessing the resources available on different nanoinformatics services or tools, all of which are searchable by category of training material, the intended target audience, the organisation that developed the training materials or by type of service, as shown in Figure 2.

Categor	у •
Target a	udience 🔹
Organis	ations involve 🔹
Service	Ŧ
Filter	Reset

Figure 2. Filters available for searching and selecting the training resources in the Library - category of training material (e.g. webinar, online tutorial etc.), intended target audience (e.g. regulator, industry, researchers), by the developing organisation or by the service type (e.g. data storage, data visualisation, data processing & analysis etc.)

³ <u>https://infrastructure.nanocommons.eu/library/</u>



On the other hand, to help the users even more, the catalogue dedicated to Services⁴ (which includes the list and the description of all NanoCommons tools and services offered via TA) allows access to the relevant training materials directly from the service page to support users in the design of their TA projects. A representative example is presented in **Figure 3**, showing the description of a service and the direct link to the resources and training materials from the NanoCommons library. In this way, users have direct access to all the resources available and can learn more on that specific tool.

A summary of the analytics on the access and user demographics regarding the NanoCommons catalogues are included in **Annex 1** (*data from 25 July 2019 until 31 Dec 2019*). More data e.g. on user demographics are included in the **Milestone 10** report.



Figure 3. Example of training resources linked to the service description. Note that TRL stands for Technology Readiness Level and relates to how close to a commercial product the tool is.

⁴ <u>https://infrastructure.nanocommons.eu/services/</u>



Description of the training activities

A detailed log of events organised or attended by NanoCommons beneficiaries, in support of the Networking Activities (NA) in WPs 2, 7, 8, 9, and 10, can be viewed <u>here</u>.

Training activities during the NanoSafety Cluster Week

Several EU projects feed their achievements (tools, models etc.) into NanoCommons for onward development (via the JRAs), as well as to provide sustainability and to enhance visibility and uptake (via the Networking activities), as per the initial vision of NanoCommons. Thus, as a research infrastructure, NanoCommons endeavors to act as a nanosafety community platform for their sustainable use and further distribution to academic researchers, industry and regulators (**Figure 4**).



Figure 4. Schematic representation on how NanoCommons connects to other EU projects and further promotes their services via its e-infrastructure and TA activities, categorised into four different stages in the nanosafety assessment workflow.

As part of its networking and community building activities, NanoCommons led the organization of the NanoSafety Week activities in October 2019 (7-11 October 2019), including the Nanosafety cluster conference, and numerous satellite training events. The week-long programme of events was coorganized by NanoCommons together with the caLIBRAte project (which held its final dissemination meeting), as well as the two nanoinformatics projects, NanoSolveIT and NanoInformaTIX (**Figure 5**). Finally, the three risk governance projects (RiskGone, NanoRIGO and Gov4Nano) held a trilateral project meeting on Friday 11th October 2019.





Figure 5. Banner of the NanoSafety Cluster week

During this event, several training activities on nanosafety-related tools (some of which are already integrated into NanoCommons, others of which may be integrated following the upcoming call for integration of external services) were included: the caLIBRAte Nanorisk governance portal, NanoSafer, GUIDEnano tool, Stoffenmanager Nano, Licara NanoScan, SimpleBox4Nano tool, nSSWD (nano Species Sensitivity Weighted Distribution), ACEnano Knowledge warehouse, and the NanoCommons data management solution.

Resources generated by NanoCommons at this event are available in the project Library and listed under the Event description⁵. The participants were asked to complete a short questionnaire in order to assess aspects about their professional experience and occupation, as well as some personal information like country and gender (see **Figure 6** for more details about this demographic analysis).

⁵ <u>https://infrastructure.nanocommons.eu/events/7/nanosafety-cluster-week/</u>





Figure 6. Statistics on the NanoSafety Cluster Week Training events participants.

ACEnano data management training

Training on THE ACEnano knowledge warehouse by Thomas Exner (Edelweiss Connect) took place on Thursday, October 10th, 2019, 13:30 - 17:00, Venue: NRCWE – Lersø Parkallé 105, 2100 Copenhagen.

The ACEnano knowledge infrastructure⁶ supports data collection, methods optimisation and knowledge sharing in the area of physicochemical characterisation of nanomaterials. While the online platform is developed by ACEnano partners, NanoCommons activities are concentrating on the integration into the NanoCommons knowledge infrastructure and on supporting the semantic

⁶ <u>https://acenano.douglasconnect.com/</u>



annotation to achieve interoperability with the NanoCommons semantic model and other NanoCommons data warehouses. Additionally, NanoCommons is in charge of the transition of the warehouse from a project-internal resource to a public data management solution allowing upload and download of data from the European and international NanoSafety communities.

The training session at the NanoSafety Cluster week, supported by both the ACEnano and NanoCommons projects, featured first the concept of distributed data management with, on the one hand, specialised data warehouses for specific data types like physicochemical, hazard, exposure and fate and, on the other hand, the semantic model to link all this data together to allow unified access to all data. Then, the specific features of the ACEnano data warehouse were presented, which uses highly structured questionnaires to document the experimental protocols including all steps and specific settings in an annotated and computer-readable way to improve reproducibility, as well as to identify differences in the results caused by small variations in the used protocols. Finally, and as the main part of the training, practical sessions on the use of the protocol questions and on the data upload workflows followed, with the participants executing all these steps hands-on using their own experimental protocols. With 15 participants, this ACEnano presentation was the second most attended training of the "Introduction to and training in the Data and NanoRisk Governance tools" session of the NanoSafety Cluster week.

The full Agenda of this training session is attached as **Annex 2**, while the materials relevant for this activity are available in the NanoCommons Library (**Figure 7**).







GUIDEnano training

The GUIDEnano tool training session was given by Socorro Vázquez-Campos (LEITAT) on Thursday, October 10th, 2019, 11:00 - 12:30, Venue: NRCWE – Lersø Parkallé 105, 2100 Copenhagen.

GUIDEnano is an interactive web-based tool that guides users in a process designed for nanomaterial risk screening, risk assessment, and nano-based risk mitigation measures. The integration of GUIDEnano in the NanoCommons knowledge infrastructure is supported by NanoCommons.

The training session at the NanoSafety Cluster week was supported by both the caLIBRAte and the NanoCommons projects. The training consisted of first a short presentation of the GUIDEnano framework including the different modules (i.e. materials, Activities, compartment/fate, Exposure, Hazard and finally the Risk Assessment and management) and the interface itself. The training was followed by a demonstration of the GUIDEnano functionality through a case study. Each registered user had access to GUIDEnano using a temporary login, giving full access to the GUIDEnano tools during a short period and enabling users to complete a pre-filled case study. After a short description of the case study context, i.e. prediction of particulate matter emissions and workers' risk in a paint factory when pouring TiO₂ NMs powder into a paint liquid matrix, the participants were guided along the different modules of GUIDEnano to understand which information needs to be filled in, and how to complete the GUIDEnano risk assessment process. Finally, the training ended with a short description of the future development and a question/answer session.



Figure 8. Impressions from the slide show of the GUIDEnano tool training.



Hackathons

Hackathon on Ontologies

9 Oct 2018 | Philip Doganis (NTUA)

The 1st NanoCommons Hackathon on "Ontological Annotation of Datasets" was co-organised by the H2020 projects NanoCommons and OpenRiskNet. The hackathon took place during the afternoon of October 9th, 2018, in conjunction with the NanoCommons Consortium Meeting (8-9 October 2018) and the OpenTox Euro Conference (8-11 October 2018) in Athens, Greece. Presentations were given by UoB Doctoral researcher Luke Slater on the structure and use of the eNanoMapper ontology^{7,8} and Dr. Dieter Meier from Biomax regarding the use of the NanoCommons Knowledge Base for the annotation of datasets^{9,10}. Following the presentations, the participants worked using their own or mock datasets and searched through established ontologies (e.g. eNanoMapper Ontology) for ontological annotations and learnt how to distinguish between similar terms corresponding to different contexts (e.g. TEM size as a data point vs. TEM as a measurement method). Participants also learnt how to prepare electronic files (e.g. JSON) containing raw data and the ontological metadata.

OpenRiskNet-NanoCommons Ontology Meeting

13-14 Dec 2018 | Egon Willighagen (Maastricht University)

The goal of this meeting was to get a picture of the ongoing ontology activities in the toxicology area, to harmonize these efforts and the developed ontologies therein, and to extend the existing toxicology ontology to support OpenRiskNet and NanoCommons tasks. Part of this was the ontological annotation of the OpenRiskNet Application Programming Interfaces (APIs) as used on their cloud. Other goals included extension of the ontology with missing terms, potentially writing up guidance documents on how to ontologically annotate datasets, and hands-on annotation of data sets (possible via OpenRiskNet data APIs). A mixed audience consisting of modellers, experimental scientists, industry and regulators participated.

NanoCommons-WGF Ontology Meeting

13 Dec 2019 | Egon Willighagen (Maastricht University)

This virtual workshop was aimed at extending the eNanoMapper ontology, now maintained by NanoCommons, towards computational toxicology. The use of OWL (Web Ontology Language) axioms is essential to this work, but the past year has shown that this concept needs dedicated workshops to disseminate this knowledge. Nine researchers from various EU NSC projects (NanoCommons, NanoSolveIT, RiskGONE) worked on OWL axioms to support computational nanomaterials descriptors, such as descriptors derived from images of nanoparticles. Furthermore, the participants worked with

⁷ <u>https://storage.googleapis.com/nanocommons/resources/2020/01/06/How_The_eNanoMapper_Ontology_Works.pdf</u>

⁸ <u>https://www.youtube.com/watch?v=rVIc_fr5R1Y&feature=youtu.be</u>

⁹ <u>https://storage.googleapis.com/nanocommons/resources/2020/01/06/NanoCommons_Hackathon_Knowledge-portal.pdf</u>

¹⁰ <u>https://youtu.be/oRhVsAFiZbl</u>



a new tool from the Birmingham team around the Manchester Syntax¹¹.

Webinars

European Materials Modelling Council (EMMC) MODA templates

26 Mar 2019 | Vladimir Lobaskin (University College Dublin)

In this internal webinar dedicated to NanoCommons members, the European Materials Modelling Council (EMMC)¹² was introduced. EMMC is a community driven bottom-up action to connect all material modelling activities and stakeholders in Europe. The mission of the EMMC is to bring materials modelling closer to the demands of industry. Further the Modelling Data Generalisation (MODA) approach and template were presented and potential areas where NanoCommons can further develop and/or promote uptake and use of the templates were discussed (**Figure 6**). The slides were made available to NanoCommons members.



Figure 6. MODA templated presented to NanoCommons members.

FAIR for NanoSafety: where do we stand?

4 Apr 2019 | Egon Willighagen (Maastricht University)

This external webinar with the US Nano Working Group (which is co-Chaired by NanoCommons coordinator Prof. Iseult Lynch) outlined the current state of FAIR nanosafety data in Europe¹³. It covered NanoCommons efforts like the continued eNanoMapper ontology development and the collaboration with the ELIXIR Training Platform and participation in the proposed ELIXIR Toxicology community. As per all presentations on this forum, the webinar was recorded and is freely available.

¹¹ <u>https://www.w3.org/TR/owl2-manchester-syntax/</u>

¹² <u>https://emmc.info/</u>

¹³ <u>https://ncihub.org/resources/2217/download/NanoWG_FAIR_Webinar_2019-04-04.pdf</u>



Nanoparticle Protein Corona Modelling Tool

25 Jun 2019 | Vladimir Lobaskin (University College Dublin)

This webinar¹⁴ gave its attendees the perspective to estimate what to expect from using the tools provided by the UCD partner through the NanoCommons e-infrastructure platform. A short Q&A session by the attendees was also included and may give further insight on the applicability of the *in silico* modeling tool for experimental researchers or students involved in nanosafety assessment. Further support to users in the application of the tools can be provided via UCD's Transnational access offer.

Protein coronas around nanomaterials (NPs) have a strong impact on the functionality and bio-effects of NPs. Interactions of biomolecules at the NP surface can be quantified and different entities can be compared. Estimations of the proteins' affinity can be made resulting in assessment of selectivity of binding of certain entities or even elucidation of preferred interaction sites. This may give rise to epitope hiding or, vice versa, an accumulation of specific epitopes (e.g. for receptor engagement) on the NP surface.



Figure 6. Webinar recording on biocorona modelling.

Use of NanoCommons infrastructure catalogues

2 Oct 2019 | Lucian Farcal (Edelweiss Connect GmbH)

An internal session was organised in order to demonstrate the catalogue functionalities, train project members on its use, and also to collect feedback. The session goals were thus to:

- Introduce the catalogues (as part of the infrastructure) to the consortium members
- Demonstrate on the catalogues functionalities and use, including issues observed so far
- Demonstrate the administration interface (for the platform administrators)
- Facilitate an open discussions on the functionalities, needs and issues.

As part of this exercise, a written tutorial (internal NanoCommons document) was prepared and shared with the project members. Also, the video recording was made available to project members

¹⁴ <u>https://infrastructure.nanocommons.eu/events/24/introduction-of-the-nanoparticle-protein-corona-modelling-tool/</u>



for further consultation. These materials will be made publicly available as the infrastructure itself is increasingly rolled out to the nanosafety research community.



Figure 7. Internal webinar on NanoCommons catalogues.

Tutorials

In addition to the webinars presented above, that generated a rich collection of training materials, additional tutorials (video or written) were made available online (**Figures 8** and **9**). Generally, these materials address user needs by presenting specific services, their use and demonstration in the form of step by step manuals. The video tutorials aim to give even more details and demonstrate the use of specific NanoCommons services or tools.

Introductory video on Nanoinformatics Model 1 Cloud Platform 9 Sep 2019	for Zeta Potential Prediction Powered by Enalos \downarrow	Video
Video clip on Guidenano tool: first insight of the 8 Sep 2019	e tool ↓	Video
Video on Enalos Nanoinformatics Cloud Platfor Nanomaterials 5 Sep 2019	rm: A Safe-by-Design Tool for Functionalized	Video
Webinar recording: Introduction to Scinote onli 28 jul 2019 → Tutorials	ine notebooks ↓	Video
Learn how to create and use a predictive mode Philip Doganis (NTUA) 15 Oct 2018	el using Jaqpot 4 ↓	Video
Learn how to create and use a biokinetics mod Philip Doganis (NTUA) 15 Oct 2018	el using Jaqpot 4	Video
Video on Modelling Nanomaterial Toxicity with NTUA team 30 May 2016	JaqPot 4	Video

Figure 8. Examples of video tutorials available in the NanoCommons Library



Tutorial for Enalos NanoXtract tool for TEM in 9 Sep 2019 → Tutorial	nage analysis	Written tutorial
Tutorial for Nanoinformatics Model for Zeta Platform 8 Sep 2019 → Tutorial	Potential Prediction Powered by Enalos Cloud	Written tutorial
Tutorial for Enalos Nanoinformatics Cloud Pl. Nanomaterials 5 Sep 2019 → Tutorial	atform: A Safe-by-Design Tool for Functionalized	Written tutorial
ACEnano knowledge infrastructure manual Oana Florean, Maja Brajnik, Lucian Farcal (Edelweiss Connect Gr 19 Jul 2019 → Manual	nbH)	Written tutorial

Figure 9. Examples of *written* tutorial available in the NanoCommons Library.

Table 1. Overview on the currently available online training tools, their formats and level ofexpertise

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



Future training activities

In the forthcoming third year, NanoCommons will set off an initiative to target the "Young Nano Scientists" of the NanoSafety Cluster. Agreements with the organisers (Nathan Bossa from LEITAT and Eva Penssler from Yordas Group) of this international group of the new research generation were made during the NSC Week in Copenhagen in October 2019. The group has regular virtual meetings about different topics of interest and relevance to the group.

The series would include the activities/services of the NanoCommons resources portfolio (<u>https://infrastructure.nanocommons.eu/library/</u>) and pursue the following aims:

- 1. To introduce NanoCommons and the TAs tools and services available
- 2. To survey what TAs the young researchers are interested in
- **3.** To make them aware and informed about the use of electronic notebooks for different types of projects (e.g. protein corona, ecotoxicology, human cytotoxicity assays, inflammatory endpoint, systems biology and work flows etc.)
- 4. To increase their appreciation of the value and use of ontologies
- **5.** To introduce predictive modelling (e.g. GUIDEnano, NTUA services, NanoFASE exposure assessment models etc.)
- **6.** To inform about the NanoCommons database facilities and how to access to support them in making their own data compliant with the FAIR data requirements.

In addition, a Face to Face event is currently in the planning phase for early 2020 in collaboration with the H2020 project GRACIOUS (Figure 10).



Figure 10. Announcement of the NanoSafety Training School to be organised in 2020

Strong participation from the NSC Work Group A on Training and Education is foreseen and hands-on training on NanoCommons services and resources shall be provided.

Currently the NanoCommons consortium is designing the online training initiative shaped for the young nano scientists, however, the chosen format shall be suitable for distributing the content further to other stakeholders, such as industry or researchers working in new member states of the EU (aligned with activities in WP2). Furthermore, a cut-down versions of two selected topics (currently under discussion by the NanoCommons consortium) shall be presented in an NCI Nano Work Group virtual meeting to participating colleagues in the US and Europe.



Conclusions

During the period covered by this deliverable (Years 1 and 2), several training activities were planned and implemented. These training activities (organised by NanoCommons and also jointly with other projects) aimed to introduce and demonstrate the capabilities of available NanoCommons infrastructure.

In order to capture and organise the information logically, a dedicated web resource was launched, which collects the description of the available services and also interlinks to the relevant resources (training materials like tutorials, presentations, video recordings, etc.) to support potential users. Therefore, the access to the services and their relevant training materials is done from a single central place. This platform will be further extended and exploited in order to cover additional requirements of the users.

The **training activities** organised recently, included the contribution to the major NanoSafety Cluster activity held in Copenhagen together with other EU projects, have been very positively received by the research and stakeholder communities. A range of supporting activities including **hackathons** and **webinars** were also organised that covered different aspects of the NanoCommons research area or its services. These activities also generated written or video **tutorials**, all made available to users in the project Library. All these training activities are successfully complementing the other dissemination activities organised by NanoCommons and presented in WP2 and WP8 Deliverables reports, and are a sustainable output and set of resources for other projects also.

Annex

Annex 1. Analytics on NanoCommons Catalogues



Co	untry	Users	% Users
1.	Greece	18	27.69%
2.	Austria	6	9.23%
3.	United Kingdom	6	9.23%
4.	Netherlands	6	9.23%
5.	Spain	5	7.69%
6.	Romania	4	6.15%
7.	Canada	3	4.62%
8.	Switzerland	3	4.62%
9.	Germany	3	4.62%
10.	Belgium	2	3.08%



ACEnano Protocols and Data Warehouse Training

NanoSafety Week, 10 October 2019 (Copenhagen, Denmark)

The aim is to introduce unique approach of the ACEnano Knowledge Protocols and Data warehouse designed to disseminate protocols and their variations and to store, manage and share data for physico-chemical characterisation of nanomaterials under standard conditions as well as at different life stages.

To improve reproducibility as well as to identify small variations in the used protocols, the ACEnano protocol system uses highly structured questionnaires to document all experimental steps and specific settings in an annotated and computer-readable way, which are then linked to the corresponding data as metadata. The training will introduce how to add protocols, create data workflows and upload data following this concept.

This will be first demonstrated by the trainer (first training slot of 1.5h) and **then executed in groups using real-world data either supplied by the ACEnano team or provided by participants from their own work** (second hands-on training slot of 1.5h). While the first is a prerequisite for the second slot, the hands-on training is optional.

Following both sessions, each participant will be familiar with the Protocols and Data Warehouse and be able to add a complete data workflow, that consists of several steps:

- 1. Add the sample preparation protocol
- 2. Add the measurement protocol
- 3. Add the data treatment protocol
- 4. Create the data workflow, including the description of the sample measured, and the protocols mentioned above
- 5. Upload raw and processed data files

Ways to increase the training experience:

- Bring a laptop in order to use it independently;
- Bring examples of protocols used in the lab for the physico-chemical characterisation of nanomaterials
- Bring examples of data files generated following the measurements (e.g. raw and processed files, calculations spreadsheets, etc.);

Agenda

	Session 1
15min	Introduction to the Knowledge Infrastructure
15min	Access to the platform, establish the cases (techniques and endpoints) covered
30min	Protocol creation
30min	Data workflow creation and upload

	Session 2
45min	Hands-on session: adding three types of protocols (sample preparation, measurement, data treatment)
45min	Hands-on session: Creation of data workflows and upload of files Discussions on eventual issues and general user experience

Useful links and resources for participants:

- ACEnano Knowledge Infrastructure: <u>https://acenano.douglasconnect.com/</u> (Signingin required)
 - Knowledge Infrastructure Tutorial: <u>https://github.com/NanoCommons/tutorials/tree/master/ACEnano manuals</u>
- Article announcing **version 1.0** of the KI <u>http://www.acenano-project.eu/news-events/34-release-of-acenano-knowledge-warehouse-data-collection-methods-optimisation-and-knowledge-sharing</u>
- Article announcing **version 2.0** of the KI: <u>http://www.acenano-project.eu/news-events/38-acenano-knowledge-infrastructure-version-2-0</u>
- Poster: <u>https://storage.googleapis.com/acenano/dissemination/events/2019/06/26/Poster_Eu</u> <u>roNanoForum_2019.pdf</u>
- For user support please contact Edelweiss Connect team at acenano@edelweissconnect.com