D10.6 - Final Version of NanoCommons Sustainability Plan

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NanoCommons

Nano-Knowledge Community

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

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Deliverable Report D10.6

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Contents

List of abbreviations

7p9 – Seven Past Nine GmbH (project partner)
AB – Advisory Board
BNN – BioNanoNet Forschungsgesellschaft mbH (project partner)
D – Deliverable
DoA – Description of Actions
EC – European Commission
ELIXIR – European Life-Science Infrastructure
ERM – European Registry of Materials
EOSC – European Open Science Cluster
EPPN – European Network for Pilot Production Facilities and Innovation Hubs
ETPN – Nanomedicine European Technology Platform a.s.b.l.
EC – European Commission
EGI-ACE – Advanced computing for EOSC H2020-funded project
EMMC – European Materials Modelling Council
ESFRI – European Strategy Forum on Research Infrastructures
EHS- Environmental Health and Safety
EU – European Union
EUON – European Union Observatory for Nanomaterials
EwC – Edelweiss Connect (project partner)
FAIR – Findable, Accessible, Interoperable, Reusable
GR – Greece
InChI – International Chemical Identifier
INISS-nano – International Network Initiative on Safe and Sustainable Nanotechnologies
IP – Intellectual Property
IRISS – The international ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes (EU project)
KB – Knowledge Base
KI – Knowledge Infrastructure
NC – NanoCommons (EU project)
NInChI – InChI for nano
NL – Netherlands
NM – Nanomaterials
NovaM – NovaMechanics Ltd. (project partner)
NPs – Nanoparticles
NRG – Nano Risk Governance
NSC – EU NanoSafety Cluster
NTUA – National Technical University of Athens (project partner)
OECD – Organisation for Economic Co-operation and Development
OITB – Open Innovation Test Bed
PLUS – Paris Lodron University of Salzburg (project partner)
RIA – Research and Innovation Action
SbD – Safe-by-Design
SSbD – Safe-and-Sustainable-by-Design
SDG – Sustainable Development Goals
SOP – Standard Operating Procedure
TA – Transnational Access
TeSS – Training eSupport System (ELIXIR's Training Portal)
UK – United Kingdom
UN – United Nations
UoB – University of Birmingham (project partner)
UM – University of Maastricht (project partner)
WG – Working Group
WP – Work Package

Introduction

NanoCommons was funded as an infrastructure project for a starting community. This means that it was supposed to build the concepts and foundation on which the community can continue to build solutions and services; in the case of NanoCommons, the infrastructure goal was to address the starting community's data and nanoinformatics needs. NanoCommons did not start entirely from scratch, as it was building on efforts of the Nanosafety Cluster's Working Group F on data management, and benefited from a general appreciation of the value of data reuse and computational predictions in the community. The push towards increasing use of chemoinforatics and nanoinformatics approaces was also endorsed by the public, regulatory and funding agencies, including being accelerated by the European ban on animal testing in the cosmetics industry and the European Green Deal. Similarly, industry are increasingly acting as a driver: fostering implementation and adoption of data harmonisation, FAIRness (Findability, Accessibility, Interoperability and Reusability of data) and openness and recognising that these activities require targeted and centralised efforts, which were provided by NanoCommons. However, a starting community is just that: a start upon which the community can build, a coalescence point around which collective efforts can nucleate. Our journey is still at the earliest stages, and much is needed in terms of automation, tooling, and continued training and education to drive the mindset changes within the community to fully embed data management at the start of the data lifecycle. Sustained and continuous support will be needed to achieve sufficient levels of digitalisation, global adoption of reporting standards both in scientific and regulatory settings, and machine-readability and machine-actionable data, all of which will lead to better quality and reproducible research, and more trust in the data and understanding of its applicability and suitability for reuse thus enhancing the value of the data and knowledge generated. This starts with sustaining what we already have, which in our case is the NanoCommons Knowledge Infrastructure, the implemented services from NanoCommons, as well as other associated partners and projects, and the collaboration with other projects established beyond the borders of nanosafety research.

The term sustainability can be described as "the ability to be maintained at a certain rate or level[1]". Applied to NanoCommons, this means that the services/tools/materials that were designed and developed during the project and are already being offered to support the nanosafety community will continue to be maintained and ideally further developed, beyond the end of the funded period of the project, ensuring future accessibility for users and potential customers. Since there will be no direct public funding for these services anymore (pending further applications via Horizon Europe for example), planning for sustainability and creation of a (not necessarily commercial) business model were started very early in the project as a central task of WP10 and possible options were continuously evaluated and adapted based on stakeholder feedback coming from surveys and, more importantly, from users of the starting infrastructure services and expertise who received support in the form of Transnational Access (TA) projects or as part of the Demonstration Cases (see deliverable reports D9.3 and D9.4 for details of the first and second round Demonstration Cases, respectively).

Deliverable D10.6 presented here builds on the previous deliverables D10.4 "First Testing and Evaluation Results of NanoCommons Sustainability Plan" and D10.5 "Second Testing and Evaluation Results on the NanoCommons Sustainability Plan", proposing the first version of the business model and analysing all

[1] https://www.lexico.com/definition/sustainability

project activities related to sustainability during the last period, respectively. Together, these three reports outline the considerations and activities undertaken with the aim of ensuring the sustained existence and utilisation of the NanoCommons project outcomes beyond the project lifetime. A major NanoCommons objective has been to achieve a sustainable and open knowledge infrastructure for the whole nanosafety community, and thus a considerable effort was invested in exploring the options and approaches, focussing on those business models consistent with the ethos of openness and accessibility, given the public funding used to develop the services, and the critical importance of access to Environmental Health and Safety (EHS) data globally. In this final deliverable, evaluation of the TAs and Demonstration Cases with respect to their (potential) contributions to the UN Sustainable Development Goals (SDGs) is completed by looking at the results from the third funding period. Additionally, the targeted activities with the strategic partners most of whom were previously identified as significant routes via which to sustain and further develop the NanoCommons tools and services, are summarised. The NanoCommons focus areas for short/long term sustainability are presented, along with the justifications of these choices. All of this information is then condensed into the final NanoCommons sustainability plan.

Description of services offered in TA projects and evaluation by TA applicants

Within NanoCommons, we have developed and given community access to services and tools in four different categories:

1. Experimental Workflows Design & Implementation: Automated data acquisition, online lab-books, data curation templates, nanoinformatics implementation.
2. Data Processing & Analysis: From data cleansing, mining and analysis to modelling and from ISA-TAB tools to ontologies.
3. Data Visualisation & Predictive Toxicity: Omics, QSARs, corona prediction, modelling and risk assessment modelling tools.
4. Data Storage & Online Accessibility: Data repositories, storage, online access.

An analysis of the categories of the TAs that have been performed during the whole lifetime of the project was carried out. From the 33 TAs that were finalised, 31 are represented in Figure 1 (the ones that were evaluated by the time of writing this deliverable). Please note that each TA may have been assigned multiple categories. Figure 1 shows that the performed TAs were not equally distributed between the 4 categories, which reflects the user demand and the efforts of the partners themselves to generate TA leads, as well as the major change in circumstances brought about by the coronavirus pandemic which meant that labs across Europe were shut for extended periods such that experimental workflows were less of a priority; notably the interest expressed by the stakeholders answering the NanoCommons Needs Survey was more equally spread (see Deliverable D10.5 "*Second Testing und Evaluation Results on NanoCommons Sustainability Plan*" for more details). We had 1 TA in Category 1, 22 TAs in category 2, 9 TAs in category 3 and 17 TAs in category 4. Most notable is the small number of applications for category 1; We assume multiple reasons for that. Firstly, some aspects of the first category have been implicitly requested in TA projects of the other categories. For example, data support, both category 2 and 4, always included some sort of defining data curation templates and sometimes also the use of electronic lab notebooks. Data visualisation and predictive toxicity projects of category 3 were not only doing the predictions but also transferring the knowhow into the group of the TA users requiring support for study design and nanoinformatics implementation. Secondly, we saw quite some confusion on what NanoCommons, as an infrastructure project, can provide as solutions for study/workflow

design and implementation when promoting NanoCommons at the different stakeholder and dissemination events. Even if we were able to explain the benefits, potential users were not always able to see directly how the concepts could be implemented in their specific setting and were, thus, not able to define specific tasks for a TA project. To change this for the future, NanoCommons dedicated multiple demonstration cases of WP9 to this area (Demonstration Case 1: Electronic Laboratory Notebooks (ELN) for data collection and annotation, Demonstration Case 4: Best-practice in nanosafety study design and its documentation via visual experimental maps, and Demonstration Case 5: Best-practice in SOP development for nanosafety assessment). This has resulted in new support tools for on-the-fly data acquisition and demonstrators on how to effectively use electronic lab notebooks, giving users more guidance. The positive effect of these demonstration cases was already seen by the increased uptake of the existing and new services within NanoCommons and associated partners working on the demonstration cases. Similar issues, albeit to a smaller extent, were seen in projects of category 2. This led, as already described in Deliverable D10.5, to partial re-defining of the awarded TA projects and extension of the allocated work effort to support the users in defining exactly what was needed and how best to implement it for their specific case.

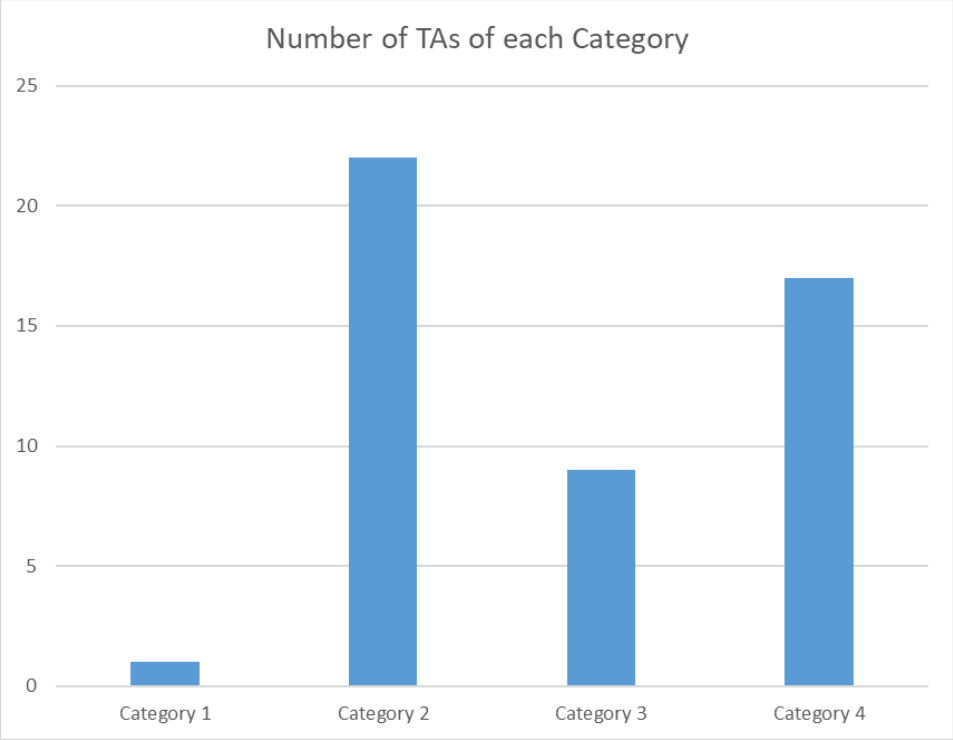


Figure 1. Number of TAs by TA category, noting that some TAs fell into more than one category, and that many projects in Category 2 also included some aspects of template design and workflow alignment (Category 1) even if not explicitly requested.

An analysis of the TA applicants regarding their stakeholder group and demographics (where they come from) has also been carried out, as shown in Figures 2 and 3. Figure 2 shows that the stakeholder group that most often applied for TAs were Universities (50%), followed by Research Centres/Organisations (28%) and SMEs (16%), in line with our expectations and with the breakdown of participants in the NanoCommons Training activities, as report in Deliverable D8.3. Figure 3 shows also the international interest in the TAs (noting that since 2016 up to 20% international applicants are allowed), having TA applicants from all over the world, with Austria (19%), Spain (13%) and the US (9%) in the leading positions.

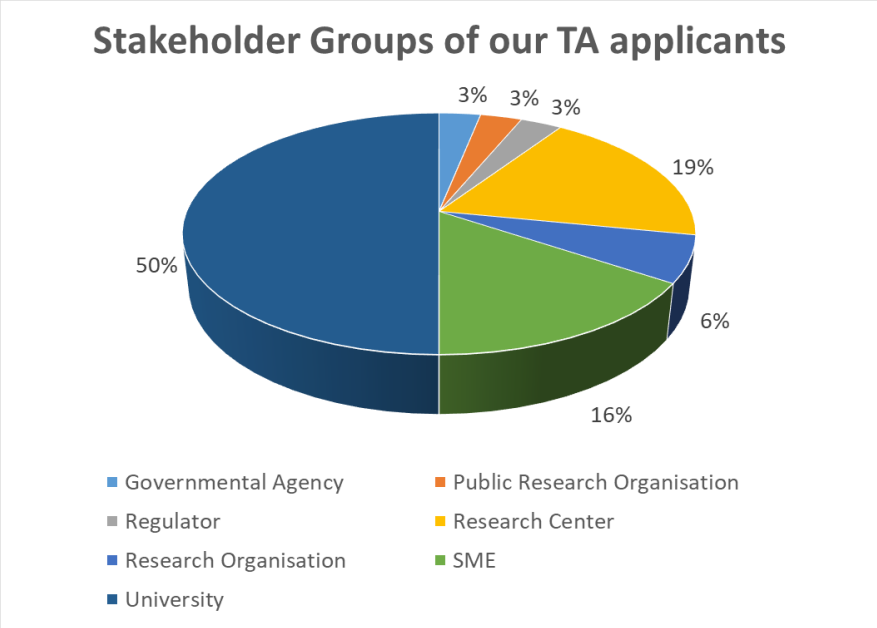


Figure 2. Stakeholder Groups of the NanoCommons' TA applicants.

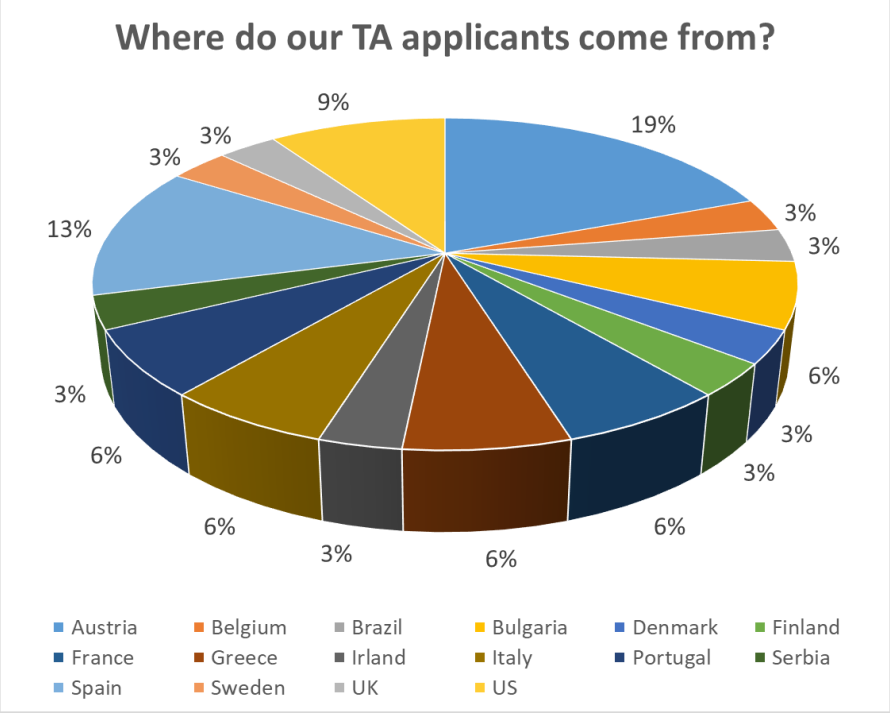


Figure 3. Demographics of TA applicants, showing the good distribution of EU countries, including new member states (Bulgaria), EU Candidate countries (Serbia) and international applicants (Brazil and US).

After finalising deliverable D10.5, 10 additional evaluations from TAs started or completed in the third funding period were received and 3 evaluations were updated, which were partly completed at the time of writing of D10.5 and now represent the full TA projects. These additional answers confirm the conclusions made in the previous report and the overall statements of the second evaluation. TA users are, in general,

satisfied with the work performed in the TAs and the benefits they received by having the chance to access (1) the expert knowledge to help them refine the research questions and select optimal approaches, (2) bespoke model development and tailoring of the NanoCommons services to their individual needs, and (3) expert input to support analysing and integrating the results. The only major outlier was a TA applied for by the SME BRAVE Analytics GmbH. They are developers of a new process analytical technology to be implemented into nanomaterial production sites. Even if upload of data produced by this technique to the NanoCommons KB was made possible, as defined as one goal of the TA project, the benefits of such an integration need still to be shown based on real-world use cases coming from BRAVE Analytics' customers using the technique in combination with other data sources. This represents one of the ongoing challenges - data management for its own sake is not sufficient but needs to lead to new opportunities baked on data accessibility and re-use. This will take some additional time to demonstrate and inevitably not all datasets will (or should) be reused, and a key challenge going forward will be helping users to determine which data have external value versus, and documenting reuse leading to additional value. How to do this remains a challenge to be tackled in follow-on projects, and is certainly not unique to nanosafety data.

Similar to what was reported in D10.5, the nanoinformatics services were able to answer the research questions completely and the results obtained are forming important parts or even constituting the main topic of joining / co-authored publications to be submitted to high-impact journals. In contrast, the experimental workflow and data management projects created more concepts and prototypes to be further developed and implemented in the institution or the project represented by the TA applicant. However, these will still be disseminated in the form of best-practice approaches or guidelines, e.g., in the NanoCommons User Guidance Handbook.

All TA providers and applicants of these new TAs agree that the NanoCommons services provide important solutions and play a significant role in reaching the UN SDGs either directly or indirectly via the results achieved by the research projects the TAs supported. However, these are mainly seen in the social and environmental pillars and less in the economic one. SDG 3: *Good Health and Well-Being*, SDG 6: *Clean water and Sanitation*, SDG 10: *Reduced Inequalities* and/or SDG 17: *Partnerships* are mentioned in almost all evaluations. Similar to D10.5, some (anonymised) quotes from the questionnaire are provided here as user testimonials (full evaluation reports are available in the deliverables of the respective TA providers, D11.1 to D20.1):

- "Some of our samples are intended for modification of membranes for cleaning water and antibacterial, antiviral applications."
- "Certainly the integration of *in silico* modelling procedures into experimental *in vitro* workflows will allow to counteract still existing data gaps in nanosafety assessment. In addition, this TA did contribute by improving data FAIRness to SDG3. In addition, the developed *in silico* techniques can be used to support product optimization for nanomedicine."
- "EU-financed open access, FAIR data reflect an enabling data donation to the global community."
- "It enables easier data sharing for research on manufactured and incidental nanoparticles in the environment, including: drinking water sources (SDG6), aquatic environments (SDG14), and soils (SDG15). The effects of data sharing are likely to lead to further insights on potential harm as well as protection measures of nanoparticles in these environments."

However, a few of the TA users have considered the commercial option for the provided services even if the amount they would be willing to pay for such services is considerably below the costs for running the TA or

they were not able to estimate acceptable amounts at the current state. Corresponding statements from the evaluation questionnaire are:

- "Developing a new methodology is a scientific process that cannot be directly linked to commercial activities, at least at its early stages. However, the re-estimated cost that is related to consulting activities around the use of the new estimation method is reasonable."
- "The actual cost for deploying a PBPK model on Jaqpot is reasonable. The service could be requested in a commercial setting."
- "Currently such costs for FAIR data are mostly not budgeted into projects, but would need to be done in future, in agreement with scientific journals [who are] more and more demanding data FAIRness; i*n silico-in vitro* experimental correlation and vice versa data enrichment is in its infancy at present. If such workflows become more often used, projects may start budgeting costs for it that may be outsourced to e.g., a commercial NanoCommons infrastructure."

In contrast, others saw absolutely no relationship of the TA to a commercial service "because scientific collaborations are beneficial for all partners involved". This broad spectrum of opinions is clearly a sign of the diversity of the TA projects ranging from applying standard services, consultancy services, collaborations to improve, adapt or even develop a completely new service, to development of concepts and prototypes. However, it also shows that NanoCommons has not yet reached a stage where all services can be offered as commercially attractive alternatives or where especially academic users see it more as a platform for scientific collaboration. While this is not surprising, given that NanoCommons is a starting community infrastructure, and will hopefully be followed-up with an Advanced Community or Design-phase infrastructure project, we note that these aspects need to be addressed before NanoCommons or any follow-on infrastructure can be run on the basis of a commercial business model only.

Demonstration case studies

In Deliverables D10.5 and D9.3, we showed that, besides demonstrating the functionalities and benefits of NanoCommons services and tools and supporting specific projects like NanoFASE, ASINA, SaByNA and ACEnano, the demonstration cases of WP9 were able to develop new ideas, explore different approaches and design new ones that enhance the infrastructure and it's services without the time pressure put on data management tasks in EU-funded Research and Innovation Action (RIA) projects. Larger conceptual changes were considered and tested already in the first set of demonstration cases (See Deliverable report D9.3), with the potential to disrupt the current way of data collection to make it more efficient and effective. Expanding on the difference between infrastructure and RIA projects further, the second set of demonstration cases was not built around specific NanoCommons functionalities but was specifically addressing broader areas identified via the online needs survey and other stakeholder engagements (see Deliverables D10.2 and D10.5), in which no solutions currently exist or where existing solutions have been identified to be suboptimal. The only two exceptions for this were Demonstration Case 7: *Grouping and read-across landscape integration* and Demonstration Case 8: *Data and informatics tools for use in nanomaterial risk assessment*. However, these were conceptualised but then postponed (to be taken up in future infrastructure or RIA projects as appropriate) and the NanoCommons consortium decided that it would be better to focus on the other cases in the limited time available. This was argued (see Deliverable D9.3) by the fact that relevant NanoCommons grouping, read-across and risk assessment features have already been demonstrated as part of WP5 and WP6. Additionally, other RIA projects are currently developing new tools,

which are not yet publicly released but are essential to be included in the demonstration cases to show the state of the art in these fields.

One area, where NanoCommons identified a critical shortage of guidelines and tools, was generation of harmonised and interoperable data integrating the FAIR principles as much as possible and at the earliest possible stage in the data life cycle. Existing data management solutions are either customised for internal usage or concentrate on long-term data storage and sharing in public data warehouses. Therefore, two demonstration cases (Demonstration Case 4: *Best-practice in nanosafety study design and its documentation via visual experimental maps* and Demonstration Case 5: *Best-practice in SOP development for nanosafety assessment*) developed ideas around data from the stages of study design, protocol/SOP development and data generation, and how existing and new tools could be combined into workflows to enable on-the-fly (real-time) data collection. Successful demonstrations on how to guide researchers in what needs to be documented and how to document it were executed. Electronic lab notebooks and the new instance map tool were essential to drive the change towards more digitalisation in the labs, where study designs, protocols, SOPs and data can be shared and discussed already during the creation process to integrate feedback and expertise from peers. State-of-the-art user management guarantees that only authorised persons have access to that data. Making the data public will then become a natural process, where more and more people can get access (paralleled by a continuous FAIRification process), instead of the currently existing strong separation between internal and public data management. In the long run, this will dramatically reduce the time effort of the researchers.

Demonstration Case 9: *Building regulatory acceptance of nanoinformatics workflows* and Demonstration Case 10: *Development of an InChI for nano (NInChI)* were also aiming at large changes in data management behaviour. The first was looking at reporting requirements to achieve regulatory acceptance especially in the field of biokinetics modelling for nanomaterials. To our knowledge, there is no example of successful use of nano-PBPK models in regulatory dossiers. This is mainly due to the lack of a standardised reporting format. The demonstration case was able to show the limitations of the existing formats just reused from other areas and what an optimal format might look like. Demonstration Case 10 was targeting the issue of missing identifiers for nanomaterials. Besides the European Registry of Materials (ERM) identifier, also developed by NanoCommons, which can be assigned to a very specific material without the need to disclose an other information, the NInChI is meant to be a structural representation (and an identifier) from which information about the size, shape, chemical composition and potentially other characteristics can be extracted, which is also aligned to the regulatory concept of nanoforms as described by the European Chemicals Agency extension to Annex i of REACH for nanomaterials[2]. Finally, Demonstration Case 6: *Support for project clusters: Safe-by-Design, risk governance, nanofabrication* aimed to solve an even more general problem of how different projects can work better together to not end up with many different incompatible platforms each providing only a subset of the tools needed to address today's challenges of risk governance, Safe-and-Sustainable-by-Design and (nano)fabrication of more and more complex (advanced) materials and products enabled by such materials. An infrastructure project like NanoCommons is in a perfect position to facilitate or even coordinate such collaboration since the focus is not mainly on new developments of tools but on providing the tools in the most optimal way, which with the triumph of cloud computing, web tools and microservices means integration into more and more complex workflows combining different functionalities,

[2] https://echa.europa.eu/documents/10162/13655/how_to_register_nano_en.pdf/f8c046ec-f60b-4349-492b-e915fd9e3ca0

from different providers / projects, to answer more and more complex research, product development or regulatory questions.

Although there is still a lot to do with all the Demonstration Cases, as well as with the activities running in parallel like training, community building & engagement, and development of the knowledge infrastructure as community tool, NanoCommons was able to start discussions, generate prototypes and (partly) full solutions, and initiate collaborations driving further developments and improvements of concepts which are able to disrupt and change current practices and replace suboptimal processes (that have traditionally resulted in limited or even lack of data reuse and, thus, lost innovative potential from publicly funded projects). NanoCommons formed, and will continue to form, the nanosafety research data landscape and will have an influence on what is seen as best-practice approaches and state-of-the-art in data management, sharing and reuse. In this way, it can be seen as the successor of the eNanoMapper and OpenRiskNet projects, which also achieved an immense impact on how the nanosafety community thinks about data with ISA-TAB-Nano, eNanoMapper database and eNanoMapper ontology being for a time synonyms for nanosafety data management and semantic annotation. More general projects like OntoCommons, GO FAIR and WorldFAIR, with the help of the domain-specific projects (nanosafety becoming part of safe-and-sustainable-by-design of advanced materials), will be able to continue the developments and activities in the EU NanoSafety Cluster and other strategic partner activities (see below) will profit from NanoCommons results and their exploitation. However, we strongly believe that dedicated infrastructure projects supporting specifically the material safety / characterisation / modelling communities will be needed to guarantee that fundamental changes in experimental, computational and data management procedures are possible also in the future when new scientific, industrial and regulatory demands require them.

Strategic partners

As part of the long term sustainability, NanoCommons' Strategic Collaborators play and will continue to play a very special role, as they act, on one hand, as multipliers of the project's outcomes and therefore, could lead to more customers by endorsing NanoCommons, and, on the other hand, provide complementary services and knowledge to be incorporated into the infrastructure. To the strategic collaborators already mentioned in D10.3[3] (i.e., ELIXIR, OECD, EUON, European Risk Governance Council and EPPN), and in D10.5 (NanoSafety Cluster, EOSC and ETPN), there are new collaborators that have been identified in the last phase of the project (GO FAIR AdvancedNano Implementation Network, IRISS, INISS Nano, ELIXIR Toxicology community, VAMAS, CODATA, PARC and WorldFAIR). The status of the recent activities and interactions with these strategic collaborators is monitored in Table 1.

Table 1. Activities with NanoCommons' Strategic Collaborators.

Strategic Collaborator	Activity / Interaction
EU NanoSafety Cluster (NSC)	The NSC, representing all European-level nano-safety related projects and being the open platform for dialogue and exchange of the European and broader nanosafety community, is still and will be the most important strategic collaborator of NanoCommons especially with respect to sustainability of the infrastructure and continuation of its operation and development.

[3] Deliverable D10.3: https://zenodo.org/record/3603179#.Yt-1uD3P2Uk

	NanoCommons is very well positioned in the NSC community due to leading roles in the NSC coordination team, secretariat and Working Groups held by different partners. Additionally, NanoCommons partners are also part of the leadership teams (coordinators or WP leaders) in different ongoing EU-funded projects associated with the NSC and can continue to promote further uptake and drive further developments of NanoCommons concepts and services via these projects. Specific activities initiated and/or matured to a level where they can stand on their own feet or be transferred to other initiatives (see below), are: Partner PLUS, responsible for the training WP of NanoCommons (WP8) and simultaneously chair of NSC WG A "Communication, Training and Education", was the driving force behind joint training activities of projects, including and often led by NanoCommons, of the NSC (see Deliverable D8.3). This drastically raised awareness and ensured high participation rates in the NanoCommons training events but also of other activities of the NSC (*e.g.,* working groups). All partners and especially UoB, UM, 7P9 and EwC were leading joint activities of the NSC and the global nanosafety community to develop, establish and promote uptake of new, advanced data management and FAIRification approaches. Major achievements in data sharing, metadata standards, ontology development, FAIR maturity evaluation and nanomaterial identifiers like the NInChI and the European Registry of Materials (see Deliverables D3.5, D4.7, and D9.4) were realised and shared e.g., in meetings of the NSC WG F "Data Management" (chaired by UM and co-chaired by 7P9) even before publication and are now adopted by many ongoing projects. NanoCommons was fostering knowledge transfer within the NSC and especially the project clusters on SbD and NanoRisk governance (see below and Deliverable D9.3). This will be continued e.g., by keeping the NanoCommons User Guidance Handbook[4] up to date, which has sections covering topics of main interest to these project clusters, the NSC and the nanosafety community in general. Currently, content from 6 ongoing NSC projects has already been published in the handbook (13 projects in total including completed as well as international projects) and content from others is in preparation.
European Open Science Cloud (EOSC)	The collaboration between NanoCommons and EOSC was successful in securing computational resources for sustaining the infrastructure and its services. With support of the EGI-ACE: Advanced Computing for EOSC project, several NanoCommons resources and services are now deployed on dedicated EOSC computing servers and will, in this way, be prepared for increased demand in the future. The computing cluster resources and their support by EwC continues to be extended beyond the end of the NanoCommons project as part of the ongoing work with EGI-ACE and EOSC.
FAIR Data Austria	The FAIR Data Austria project[5], led by the Technical University Graz, is designed to strengthen knowledge transfer between universities, industry, and society

[4] NanoCommons User Guidance Handbook: https://nanocommons.github.io/user-handbook/
[5] FAIR Data Austria project webpage: https://forschungsdaten.at/en/fair-data-austria/

	and supports the sustainable implementation of EOSC. Therefore, during the last period of the project, a connection was established, which brought one successful TA application (TA29) to generate a prototype and a hands-on showcase of a (semi)automatic workflow to make FAIR data publicly available in the public institutional repositories (e.g., of universities) and in the NanoCommons Knowledge Base as the central place to access nanosafety related data. This semi-automatic workflow is a first step in the automation of the process, including resource savings and on-the-fly FAIRfication of data (metadata and data harmonisation,...) and this work will be continued to generate general solutions usable by all partners of FAIR Data Austria and potentially also in other scientific areas.
ELIXIR & ELIXIR Toxicology Co mmunity	ELIXIR, as the infrastructure for the life-science community aims to sustainably link, allocate, manage, safeguard and provide all relevant data as well as data manipulation and modelling tools. Even if nanosafety is a community of it own right and requirements, the overlap with the larger life-science community is obvious[6] and was used to promote NanoCommons events / webinars / workshops and offer related training materials on TeSS, ELIXIR's Training Portal with the goals of reaching a wider community and helping to extend NanoCommons' and ELIXIR's user base. Knowledge exchange between the two communities was also fostered by NanoCommons actively involved in ELIXIR's organising structure, e.g., UM as member of ELIXIR-NL, UoB of ELIXIR-UK, NTUA of ELIXIR-GR and 7P9 as a member of the Industry Advisory Board. One continuing collaboration with ELIXIR is the work and adoption of Bioschemas as an interoperability solution for making data and knowledge more FAIR. NanoCommons has developed the ChemicalSubstance profile, following the MolecularEntity profile, but for nanomaterials. Bioschemas annotation has been added to various NanoCommons pages, such as the *Ontology IRIs for the JRC representative industrial nanomaterials*[7] and the *Overview of open datasets released by NanoSafety Cluster projects*[8]. The most important new development was establishing the new ELIXIR's Toxicology community, which was driven by partner UM with the support of partners 7P9, UoB and NTUA. The goals of this community focus on bringing the life science, nanosafety as well as chemical safety communities closed together by reusing each others approaches and tools and continue to harmonise data and make it interoperable and computer-actionable across all three communities[9].
GO FAIR AdvancedNano IN	The Advanced Nano FAIR Implementation Network (IN) was established within the GO FAIR initiative by the EU project Gov4Nano in October 2020. Its high-reaching aim is to actively support the implementation of the FAIR principles in

[6] Karcher S. et al. Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. NanoImpact, 2018, 9, 85-101. https://doi.org/10.1016/J.IMPACT.2017.11.002
[7] https://nanocommons.github.io/specifications/jrc/
[8] https://nanocommons.github.io/datasets/
[9] Martens, M. et al. ELIXIR and Toxicology: a community in development. F1000 Research, 2022, https://doi.org/10.12688/f1000research.74502.1

	the current nano-Environment, Health and Safety (nanoEHS) databases (i.e., data on NM physico-chemical characteristics, release and exposure, toxicity and functionality). The Advanced Nano IN profited from the active contribution of several members of **NanoCommons** (BfR as co-lead, UoB, UM, 7p9) in providing the experience gathered from the infrastructure project. Likewise, the Advanced Nano IN aims to fulfil the gaps and needs identified by **NanoCommons**, regarding data reuse, and this endeavour gave life to most of the Advanced Nano IN activities. The goal of the Advanced Nano IN is to connect these stakeholders in the field of nanosafety and to provide them with guidelines towards FAIRification of their datasets and databases. An alliance/network for FAIR data is needed to take new, ground-breaking steps in the nanosafety domain, specifically in the areas of grouping and read-across, hazard and risk assessment, Safe and Sustainable by Design, development of *in silico* approaches (e.g., QSARs) and development of Adverse Outcome Pathways. Although the nanosafety community is in an advanced stage in terms of FAIR data, clear rules for its sustainable implementation, improving FAIRness and data reuse are still a matter of development. The role of the AdvancedNano IN is to outline and execute an action plan towards fulfilling these missing aspects. Importantly, activities of the AdvancedNano IN also included the outreach to other projects, where clearly **NanoCommons** was a fundamental project and a key partner. In close collaboration of NanoCommons and Gov4Nano, a map of FAIR activities was created to get an overview on all major activities from the different EU-funded project (see D9.4 for details). For this purpose, a detailed questionnaire was developed and circulated among all major EU nanosafety projects. The three NMBP-13 risk governance projects Gov4Nano, NANORIGO and RiskGONE, the research projects NanoSolveIT, NanoInformaTIX, CHARISMA and smartCERIALS, and the infrastructure project **NanoCommons** provided information. This initiative also reached out to national projects such as the German National Research Data Infrastructure project NFDI4Cat, which provided insights into the implementation of the FAIR principles in another domain, still partially connected to nanomaterials. In addition, several individual follow-up teleconferences took place, to discuss in detail the FAIR activities of the various projects.
Organisation for Economic Co-operation and Development (OECD)	NanoCommons has actively supported addressing data and nanoinformatics related issues of the Malta Initiative[10]. Originally, this was planned to be performed within the Industrial Case Study 3 (on the extension of skin sensitization assessment methods to nanoforms) and 5 (defining vocabulary for OECD guidelines that can be used in NanoCommons applications supporting assessment and testing nanoforms). However, because of the cancellation of the Industrial Case Study programme due to complications in the negotiations with the industry partners, a more indirect collaboration with the NanoHarmony project, as one of the funded projects in charge of developing test guidelines for

[10] The **Malta Initiative** is a European Action to develop OECD Test Guidelines for NMs and aims to develop and amend the test guidelines (TG) and guidance documents (GD) to ensure that nano-specific issues for fulfilling regulatory requirements are addressed.

	the Malta Initiative, and the OECD was established. A collaborative dialogue between NanoCommons and the WP1 Task leaders in NanoHarmony was initiated aiming at ensuring that the OECD Technical Guidelines and Guidance Documents being developed in NanoHarmony WP1, as well as related documents are produced and reported compatible for further use. OECD TGs should not only deliver internationally valid data through the OECD Mutual Acceptance of Data protocol, but also adhere as closely as possible to the guidance and checklists for experimental data (as e.g., outlined in NanoCommons D6.1 Annex 2 "Checklist for NanoCommons workflow for Risk Assessment"), thus also making the data as fit for inclusion and use in the future computational risk assessment tools for which the foundations are being developed in NanoCommons, as is possible.
European Union Observatory for Nanomaterials (EUON)	NanoCommons has entered a TA with the EU Observatory on Nanomaterials (EUON) to interface the EUON Infocards and the NanoCommons Knowledge Base (NC KB). A use case requirements analysis was jointly executed and corresponding technical solutions designed. Specifically application programming interfaces (APIs) to search the NC KB and retrieve information where provided to EUON based on native NC KB data formats. In addition the IUCLID format proposed by EUON as a standard for data exchange was analysed and semantically mapped to the NC KB format. Access to the EUON Infocards API was provided by EUON and analysed for integration with the NC KB. Based on the TA results NanoCommons can be made visible on the EUON webpage to support the long term exploitation of project outcomes, and work is ongoing to achieve this as part of the sustainability activities.
Organisational Forum of the Nano Risk Governance – Risk Governance of Nanomaterials: 3 European Projects Working Together: Gov4Nano & NANORIGO & RiskGONE	To boost the effectiveness and synergies between the funded projects addressing governance and nanoinformatics, an interaction commitment between the projects Gov4Nano, NANORIGO and RiskGONE has been agreed. These three projects are developing an Organisational Forum for Nano Risk Governance (called the Nano House to visualise a community structure where each room will support different aspects of Nano Risk Governance (NRG) such as data management, informatics tools, measurement protocols and Standard Operating Procedures (SOPs) and pre-validation activities etc.), with a Nano Risk Governance Framework underpinning the activities and efforts, to support industry (especially SME) and regulatory decision making. An inter-project core group on data management has been formed (Chaired by NanoCommons Coordinator Iseult Lynch, WP Leader for ecotoxicity in RIskGONE) that will link the NanoCommons Knowledge Infrastructure with the NRG portal and framework. NanoCommons is feeding directly into this and supporting the development of the decision support tools for the Nano House, and the integration of datasets and tools to facilitate risk assessment. In the Nano House, tools and data management will play a key role, and therefore this collaboration is very relevant for the long-term sustainability of NanoCommons project outcomes.
Nanoinformatics Projects: NanoSolveIT	NanoSolveIT & NanoCommons are already a nanoinformatics hub for all past and ongoing efforts in harmonising and unifying nanosafety datasets (through

& CompSafeNano	NanoCommons & NanoSolveIT Knowledge Bases and the nanoPharos database). Furthermore, several nanoinformatics models are co-developed and hosted on both cloud platforms with user-friendly graphical user interfaces specifically designed for stakeholders with different levels of expertise. CompSafeNano has been designed as a convergence science project to truly integrate existing nanoinformatics (e.g., NanoSolveIT and NanoCommons) and nanomaterials governance projects (RiskGONE), and bridge gaps in methodologies and approaches as proposed by the Nanoinformatics Roadmap, by fostering mutual learning, innovative collaborations, and a trans-disciplinary and trans-sectoral language and knowledge integration. CompsafeNano will continue to develop the tools and approaches through 2025.
European Network for Pilot Production Facilities and Innovation Hubs (EPPN), SUSNANOFAB, NanoFabNet Hub, open innovation test beds (OITBs)	In the beginning of the project (2018-2020) NanoCommons interacted with the EPPN in order to share its know-how and help the pilot projects in bringing their research to the next level, addressing interesting topics for individual projects or collectively via the EPPN. The activities started by the EPPN community are continued to a certain extent. However, beyond EPPN, other projects are sharing knowhow in different ways: 1) SUSNANOFAB has included the EPPN in their project work; 2) NanoFabNet has developed a web-platform that will exist in the long-term as a supportive hub on sustainable nanofabrication, interacting with data infrastructures like DaNa[11] and NanoCommons; 3) projects developing process analytical technologies for industrial nanomaterial productions like NanoPAT, NanoBAT, etc., have included metadata-tasks to contribute to knowledge exchange; 4) Open innovation test beds like NextGenMicrofluidics, FlexFunction2Sustain, etc., established interaction links with the EU NanoSafetyCluster to connect with the NanoCommons and other nanoinformatics experts in specific domains (e.g., microfluidics). NanoCommons actively supported the development of concepts and implementation for the digitalisation of processes and real-time data management. This included sharing expertise collected during the management of data of large projects especially with tools for on-the-fly data collection and integration of distributed data sources. This was complemented by alignment of and mutual invitations to training activities and development of common concepts for the future provision of community platforms and knowledge resources. As one direct result supporting the sustainability of both projects, formal collaboration with and involvement of NanoCommons partner 7P9 in the NanoFabNet Hub, the knowledge and community platform for nanotechnology professionals and entities, was established allowing users of the hub to profit from the complementarity of expertise of the two consortia.
Nanomedicine European Technology Platform (ETPN)	Dissemination and promotion actions of the NanoCommons project via the ETPN association took place during the last period of NanoCommons, enhancing the chance of collaboration and interaction with more projects and, at the same time, making a step forward to interlinking both nanosafety and medicine

[11] see webpage: https://nanopartikel.info/en/

	communities. NanoCommons online training sessions were promoted within the ETPN bench community including the nanoinformatics and data management tools, modelling and risk assessment services. We note of course that nanomedicines have specific reporting and quality requirements beyond those of other chemicals, and as such direct transfer of all approaches may not be possible, but there is enormous scope for mutual learning, and indeed many of the issues addressed, such as characterisation, assessment of toxicity etc. are common. Indeed, a new Horizon Europe MACRAMÉ brings together partners from NanoCommons and from the lasagne nanomedicine project REFINE to progress approaches together, with the data management approaches inspired by NanoCommons.
IRISS	The recently started EU Horizon Europe project IRISS (*The international ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes*) aims to accelerate the transition to safe and sustainable materials, products and processes. Several NanoCommons partners (BNN, UoB, NTUA) are involved in IRISS, ensuring that NanoCommons efforts for the digitalisation and FAIRification of processes (via data management and nanoinformatics tools) are included in the IRISS developments since the beginning of the project. With its broader scope, IRISS will become an important link between all relevant stakeholders in material research including nanomaterials, benefitting from the NanoCommons infrastructure and its integration into the larger materials ecosystem. The interactions towards road-mapping, working along different value chains and across SSbD-parameters will create opportunities to apply NanoCommons assets. In the long run, this shall support the ambition of NanoCommons to become a part of the fundament of the European nano-data-ecosystem, which might be also part of the future strategic outputs of IRISS.
PARC	The €400 million Partnership for Assessment of the Risks of Chemicals (PARC) is a public-public partnership to accelerate the modernisation of current approaches to chemicals regulation, focussing on integration of New Approach Methodologies (NAMs), application of approaches for assessment of mixtures of chemicals, and integration and harmonisation of disparate data on human and environmental exposure, human and environmental hazard and risk assessment. While PARC is not focussing on nanomaterials in particular, the leadership and approaches developed in NanoCommons to emphasis the need for data management to occur much earlier in the data lifecycle, i.e., at the point of experimental planning and data capture, and the need for and role of the data shepherds to support data generators and data curators to reach common understanding, have been implemented into PARC. UoB are the co-lead of PARC WP7 on FAIR data management, and will ensure that NanoCommons approaches are embedded and built into the sustainability planning of PARC, which includes integration with the IPCHEM database (currently focussed on exposure monitoring but its further development by the European Commission will include toxicology and risk also).
INISS-nano	The INISS-nano initiative (*International Network Initiative on Safe and*

	Sustainable Nanotechnologies) arises from the EU-Asia Dialogue on NanoSafety (organised by members of the NSC and the Asia Nano Forum). It prepares the ecosystem for global collaboration in selected fields of action: (i) Harmonisation, (ii) Support industrial understanding, (iii) Sharing / facilitate sharing of resources/ infrastructures, and (iv) Ethical aspects, enabling "collaboration without borders" within joint projects, joint funding initiatives, and any further way of cooperation. Based on the idea of a "network of networks", it was formed to bring together science, industry and government from partners all over the world, not duplicating structures but connecting with them (e.g., NSC, ANF, EC & JRC, EU-US Communities of Research (CoRs), standardisation bodies (such as CEN, ISO, ASTM, etc.), OECD & BIAC, ECHA). The focus of INISS is on the collaboration in different fields pertaining to nanotechnology research in general and nano-safety research in particular. This shall include collaboration in terms of training, standardisation efforts, test-guidelines development, metrology, commercialisation, ethical aspects, sustainability, and joint research, supporting governance, regulatory guidance, and, of course, being open for further joint working items[12]. Several NanoCommons partners are involved in the INISS-nano initiative, ensuring that this global collaboration is based on the efforts on digitalisation, harmonisation and FAIRification of data and processes (via data management and nanoinformatics tools) developed in NanoCommons.
IUPAC and InChI Trust, CODATA, and VAMAS	The development of the line identifier for nanomaterials, the NInChI, was the starting point for intensifying the collaborations with these global chemical nomenclature and terminology, open-data and open-science, and pre-validation organisations. More information and involvement in the NInChI is described in Deliverable D9.4. Each organisation now has its own working group, task group or project, which in the case of CODATA already received additional Horizon Europe funding. Even if the funding is relatively limited, the combined influence and the achieved visibility will guarantee that the development of the NInChI will be continued by a global group of stakeholders. However, the interactions with these organisations also allowed identification of additional potential collaborations apart from NInChI: 1. CODATA and VAMAS were working on the Uniform Description System (UDS) for Materials on the Nanoscale, which was used as the basis to identify the characteristics to be encoded in the NInChI. The NInChI groups work on integrating the NInChI into this standard either as addition or to substitute information requirements, which are covered in the NInChI. Activities will then be started to transfer these changes into the standards based on the UDS and potential other standards. 2. IUPAC has started activities for developing a naming convention for nanomaterials. These can profit from the expertise collected with the NInChI and vice versa and knowledge exchange between the two groups has already started. 3. As described in Deliverable D17.1 (TA project NC30), there is the need

[12] Falk et al. (2022). INISS-Nano: revised concept and action plan (International Network Initiative on Safe and Sustainable Nanotechnologies) (Version_02). Zenodo. https://doi.org/10.5281/zenodo.6818049].

	for a standard for better description of data coming from real-time monitoring devices and how to combine them with other data sources. First discussions with VAMAS as well as with ISO have been initiated to secure their support for these developments. 4. Expertise from NanoCommons, especially from its collaboration with the ACEnano project, could be used to create a general system to support data collection and sharing from round robin or Interlaboratory testing. Design of specification for such a system has been started in collaboration with VAMAS.

Raising awareness of the contribution of FAIR nanosafety data to the UN Sustainable Development Goals (SDGs)

As already indicated in deliverable D10.4, the UN SDGs present guidelines for organisations or projects such as NanoCommons to develop, implemente and provide services in a manner fostering economic, environmental and social sustainability directly by the transition towards a more digitalised and collaborative way of undertaking (nanosafety) research and sharing openly and FAIRly the resulting datasets to allow their re-use globally. In addition to the data itself, the web-based platforms provided for each of the tools and services supports equitable access to them and enables users to apply them without needing a background in modelling or programming, such that they can be utilised by regulators and small industries globally to improve health and environmental conditions.

To evaluate how NanoCommons has been supporting the achievement of the SDGs through its research support services, and how these services are essential for development of safe and sustainable nanomaterials (NMs) and nano-enabled products, and more broadly will have a positive impact on the “global innovation system” for the sustainable development of new technologies, both TA providers and users were surveyed as described in Deliverable D10.5 and complemented with the period 3 TA project evaluations as described above. Figure 4 shows the main SDGs that NanoCommons expected its activities to address, based on the preliminary analysis by UoB and BNN which was presented in Deliverable D10.4.

Figure 4. SDGs mapped to the three pillars of sustainability that were expected to be addressed either directly or indirectly through the research and development activities of NanoCommons (as shown also in deliverable D10.4).

From the first replies to the survey of TA project users and providers, we noted that there was some uncertainty on how to relate the work performed and the obtained results to the SDGs, both on an individual TA level but also on the level of the broader impact of the supported projects and similar projects benefiting from the NanoCommons services. This led many NanoCommons partners to ask for more training on the SDGs and what the sustainability WP (WP10) had in mind for this activity. In order to address these needs and to support the partners in the task of identifying which SDGs have been addressed in the different services being offered by the project via the TAs, an internal, interactive webinar on SDGs was organised by BNN, on 9th May 2022. It created a common understanding on the term "sustainability", put sustainability and the SDGs into a wider context, and created awareness and understanding regarding how open and FAIR data, tools and models supports the achievement of the UN SDGs. The webinar started with a presentation by Clemens Wolf to set the scene on the specific topic. The aim of this presentation was to highlight the importance of addressing the SDGs with our research and to increase the consortium's knowledge on the different aspects addressed by the SDGs within the nanosafety community. This was followed by an interactive open discussion, moderated by Susanne Resch. An online white board, MURAL - see Figure 5, was used to facilitate the interaction of all NanoCommons partners and to stimulate their active participation while answering the following questions:

- Q1: Which UN SDGs are relevant for NanoCommons from your point of view? How do open/FAIR data, tools and models support the SDGs? What are potential barriers and challenges?
- Q2: How can open and FAIR data, tools and models support the achievement of specific SDGs?
- Q3: What is needed to make this happen (1 +2)?

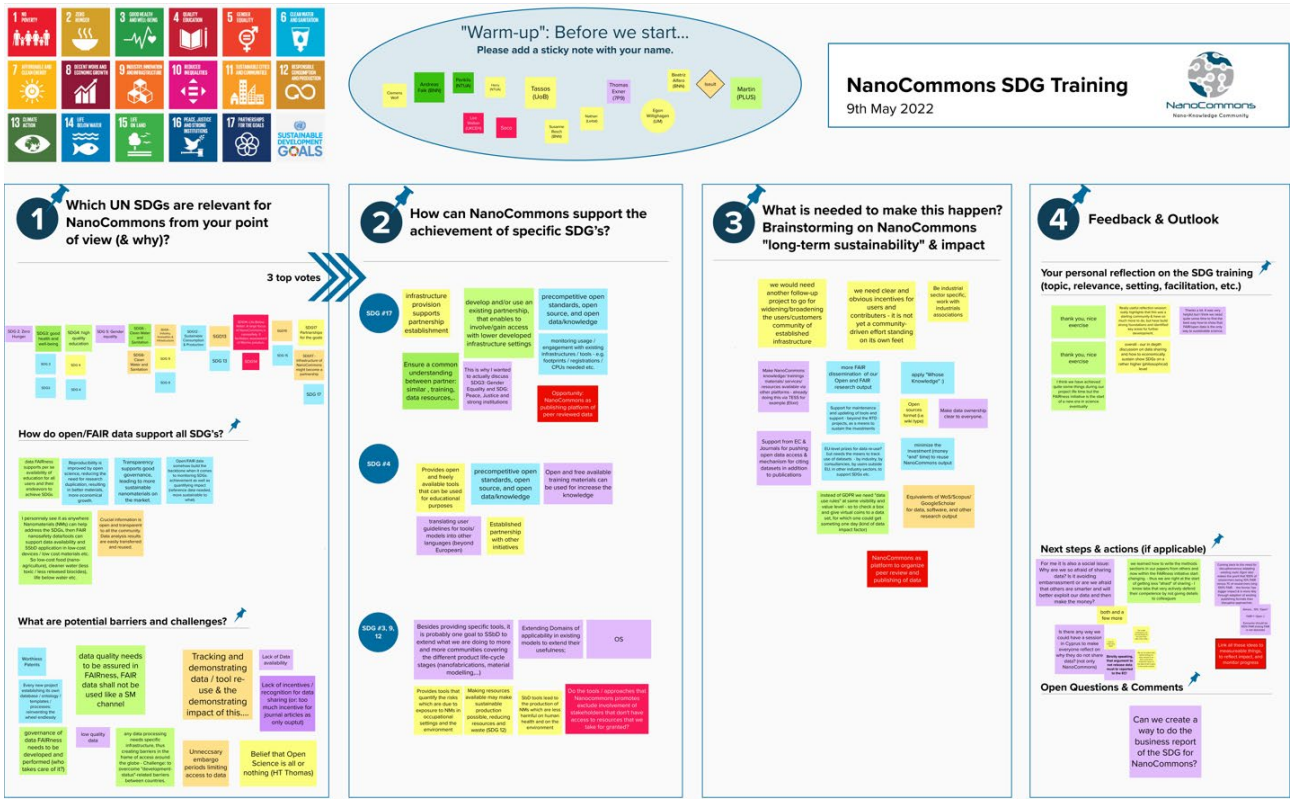
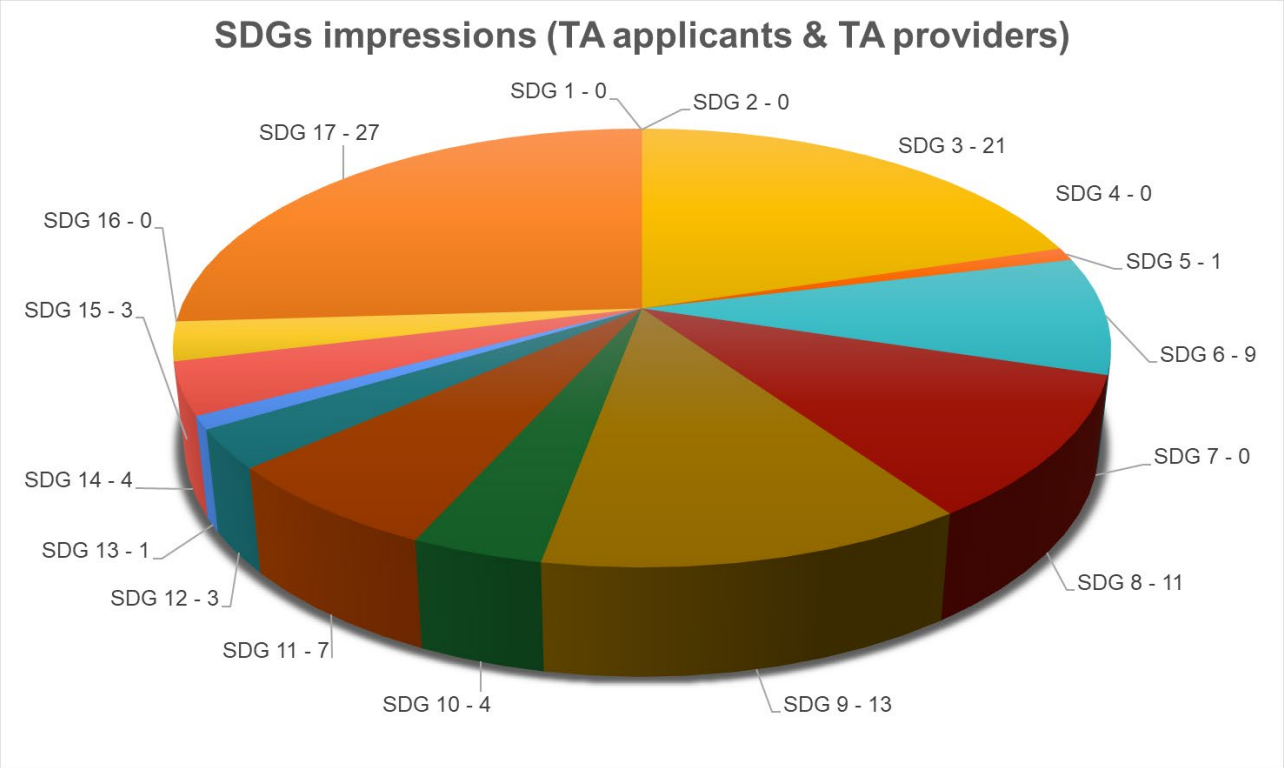


Figure 5. Outcome MURAL of the Internal workshop addressing the UN SDGs.

The workshop was very well received and the learnings from the workshop were included in the last round of evaluations of the TAs of the third funding period. Furthermore, the workshop and the 1-to-1 meetings with the TA providers helped NanoCommons partners think more broadly and better understand and identify the SDGs addressed in their own work, as can be seen in Figures 6 and 7. Figure 6 shows an overview, from both the TA providers and TA applicant perspectives, of the SDGs that were identified as being addressed in the different TAs implemented and evaluated during the whole life-time of the project. Many SDGs have been addressed, as they are partially interrelated. Some SDGs like SDG 3 "Good Health and Well-Being" and SDG 6 "Clean Water and Sanitation" are quite obvious since they are directly related to nanosafety. However, it is very encouraging that SDG 17 "Partnerships for the Goals", was actually the most often named SDG, with SDG 9 "Industry Innovation and Infrastructure", and SDG 8 "Decent work and Economic Growth", and to a lesser extent SDG10 "Reduced Inequality" and SDG11 "Sustainable Cities and Communities" also being identified frequently in the TA project evaluations. This demonstrates that NanoCommons was successful in its mission of being a community building initiative and in providing a nanosafety data and nanoinformatics infrastructure available to many. This correspondence between mission and results/impact can also be seen by comparing Figure 4 (our pre-analysis) and Figure 7 (post-evaluation by the TA providers and users). All expected SDGs were addressed but also less obvious SDGs were associated with the TA projects following the evaluations by Users and providers, which can be reasoned by the larger awareness of these goals through participation in the NanoCommons SDG workshop and increasing awareness generally as many journals and publishers are increasingly tagging articles with specific SDGs, further building awareness. For example, Elsevier have special issues dedicated to specific goals[13], and a tracker for the number of

[13] https://www.elsevier.com/connect/how-societies-and-their-journals-can-support-the-un-sdgs

publications in each goal over the previous month[14], while Springer Nature have an SDG programme and Communities and recently conducted a survey of researcher attitudes to each of the SDGs [15], the raw data from which is available to download into Jupyter notebook for further analysis. Indeed most publishers have signed up to the SDG Publishers Compact[16] which aspires to develop sustainable practices and act as champions of the SDGs during the Decade of Action (2020-2030), publishing books and journals that will help inform, develop, and inspire action in that direction. Given the low awareness identified among NanoCommons collaborators on how their research is supporting the SDGs, we will publish the NanoCommons analysis of the SDGs and how open and FAIR nanosafety research is progressing these as a Commentary or Perspective type article in the literature (in progress).



SDG1: No Poverty
SDG2: Zero Hunger
SDG3: Good Health and Well-being
SDG4: Quality Education
SDG5: Gender Equality
SDG6: Clean Water and Sanitation
SDG7: Affordable and Clean Energy
SDG8: Decent Work and Economic Growth
SDG9: Industry, Innovation and Infrastructure
SDG10: Reduced Inequality
SDG11: Sustainable Cities and Communities
SDG12: Responsible Consumption and Production
SDG13: Climate Action
SDG14: Life Below Water
SDG15: Life on Land
SDG16: Peace and Justice Strong Institutions
SDG17: Partnerships to achieve the Goal

Figure 6. SDGs identified as being addressed in the different NanoCommons TA projects (based on the TA evaluations from the TA applicant and TA provider perspectives).

[14] https://sdgresources.relx.com/
[15] https://www.springernature.com/gp/researchers/sdg-programme
[16] https://www.un.org/sustainabledevelopment/sdg-publishers-compact/

Figure 7 represents the SDGs addressed by NanoCommons in the three pillars of sustainability, taking into account the opinions of TA providers and applicants in the TAs that have been evaluated. It can be seen that it is quite similar to Figure 4, where the expectations were presented. After the evaluation, some SDGs were newly identified (SDG3, SDG10, SDG11 and SDG15), while SDG16 disappeared from the scene (in part due to the fact that our tools and approaches are quite early stage and have not yet been validated for use in risk governance for example). This representation is purely qualitative and does not reflect the relative proportions of the TA projects and NanoCommons partners addressing each SDG quantitatively. For this more quantitative view please refer to Figure 6.

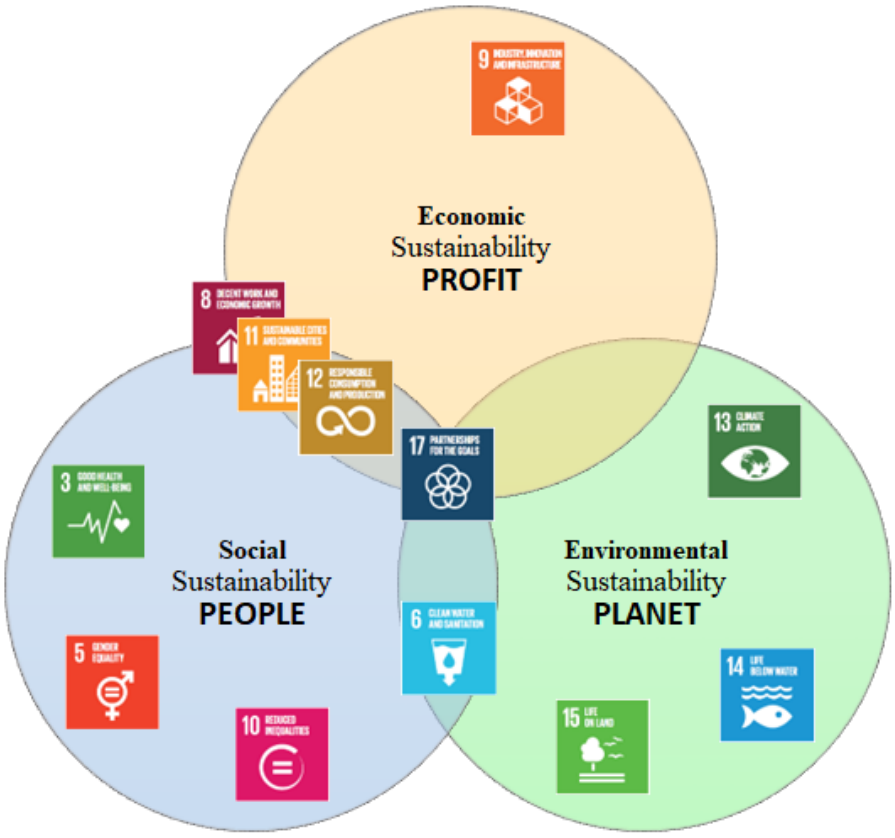


Figure 7. Representation of the SDGs identified as being addressed in the different NanoCommons TA projects (from the TA applicant and TA provider perspective).

Short/long term sustainability of NanoCommons

NanoCommons has achieved the provision of services and user support in many fields: development of data concepts including the "data shepherd", that has been adopted by different projects (e.g., ASINA[17]), public availability of data and nanoinformatics services and tools (via the Knowledge Base and Knowledge Infrastructure), development of several TAs, preparation of training materials and organisation of lots of workshops/webinars/hackathons. These services have now to be sustained, which includes not only

[17] https://nanocommons.github.io/user-handbook/data-management/data-shepherds/ASINA-data-shepherd/

maintenance but also further development and extension of the functionality to keep the infrastructure relevant and up-to-date. Since there is no direct follow-up project, sustaining NanoCommons and its set values need to be continued in the short term as a community activity, actively driven by the NanoCommons partners via their involvement in strategic partner activities like the ELIXIR Toxicology community, GO FAIR AdvancedNano IN, InChI Trust, INISS-nano as well as H2020 funded projects like NanoSolveIT, RiskGONE, SaByNa, SABYDOMA, ASINA, CompSafeNano, Diagonal, and Horizon Europe funded projects such as PARC, IRISS, INQUIRE and WorldFAIR (as well as forthcoming project MACRAMÉ). We hope that we can, in this way, reproduce the success of the eNanoMapper project, which ended in 2017 but whose main outcomes (eNanoMapper database and eNanoMapper ontology) continue to be used and improved in many other projects not only in Europe but globally.

To make the need for sustainability and community adoption of the NanoCommons outputs visible to the wider community as the H2020-funded period ends, NanoCommons partners decided to rebrand from NanoCommons being an infrastructure project to NanoCommons being the *Nanosafety community infrastructure.* This transition was also signalled visually by slightly modifying the logo as well as separating the community resources offered by NanoCommons infrastructure from the project website in terms of colour. The new logo can be seen in Figure 8 with the colours being refreshed, going from a "NanoCommons project" blue into a "NanoCommons sustainable community" green (see Annex I for the brand guidelines). The sustainability plans and rebranding were highlighted in different sessions during the Nano-week 2022 & NanoCommons Final Conference in Cyprus with a talk by Iseult Lynch, the TA presentations and the NanoCommons training activities, while the support by the strategic partners and the ongoing projects, even those without direct involvement of NanoCommons partners, was secured in personal interactions throughout Nano-Week 2022 (20-24th June 2020) in Cyprus which was organised by NanoCommmons in conjunction with the NSC projects.

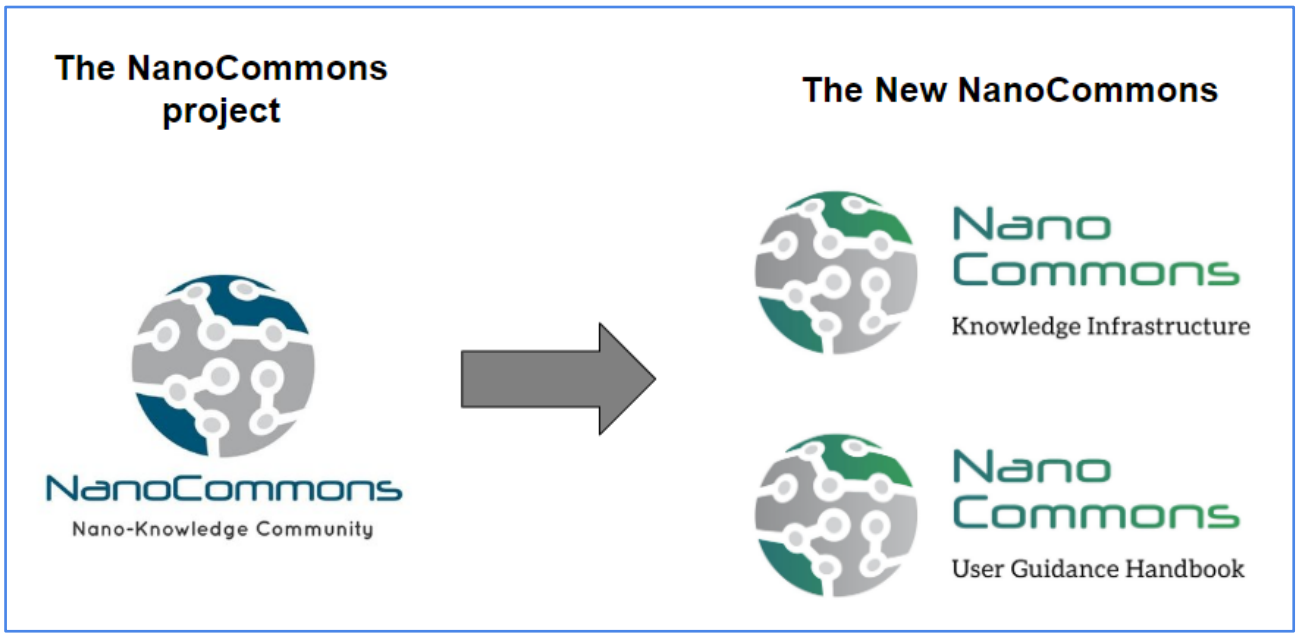


Figure 8. Old vs. New Logos reflecting the change from NanoCommons funded project to NanoCommons Knowledge infrastructure as a community driven and sustained platform.

Even if funding via different projects will guarantee the existence of the nanosafety infrastructure, in the longer term, additional funding for specific follow-up projects concentrating completely on the infrastructure development will be needed to be prepared for the new challenges coming from the European Green Deal and the Chemicals Strategy like moving from nanomaterials to advanced materials and integrating nanosafety into concepts representing the full material and product life cycle and following Safe-and-Sustainable-by-Design paradigma. Discussions have been started in the broader community to define the role of this extended infrastructure (completely virtual continuing to focus on data and computational tools or mixed including also experimental testing) and with national representatives to get their support. Even if all these discussions are still ongoing, the current state clearly shows that there is a broad agreement on the need for such an infrastructure and the next steps will be a more concrete planning of the next steps, which should finally lead to applying to become part of the next European Strategy Forum on Research Infrastructures (ESFRI) Roadmap having previously secured all national support needed for a successful application.

Foundation for both, short- and long-term sustainability, will be the 4 areas (described in further detail below), in which NanoCommons achieved major break-throughs and where our services were highly demanded as part of TA projects or other sorts of collaborations between NanoCommons and individual researchers or publicly funded projects:

1. NanoCommons Knowledge Base and Data Warehouse
2. NanoCommons User Guidance Handbook
3. Nanoinformatics Tools & Services
4. Training materials.

1. NanoCommons Knowledge Base

The NanoCommons Knowledge Base (KB) and Data Warehouse (DW) were successfully established as an important data resource of the NanoSafety community. The start screen of the KB is shown in Figure 9. Different projects as well as individual groups are using them for long-term storage of the generated data. Perhaps even more importantly, integration of metadata from the other important data warehouses in the field (eNanoMapper, ACEnano, RDF version of the AOP-Wiki) was achieved through semantic linking, which renders the NanoCommons Knowledge Base as a one-stop shop for searching data from across all these data resources, with direct links to the original resources for access of the data. In this way, researchers benefit from a common search interface combined with access to specific features for data visualisation, analysis and aggregation provided by the other databases and specifically designed for one kind of data. For more information, please see Deliverable D4.7 which provides full details of the final implementation of the NanoCommons Knowledge Base. The NanoCommons KnowledgeBase will be sustained jointly by Biomax and UoB as part of the NanoSolveIT project, and Biomax have committed to an additional 5 years of support for the KNowledge Base as part of its developmental activities in this area.

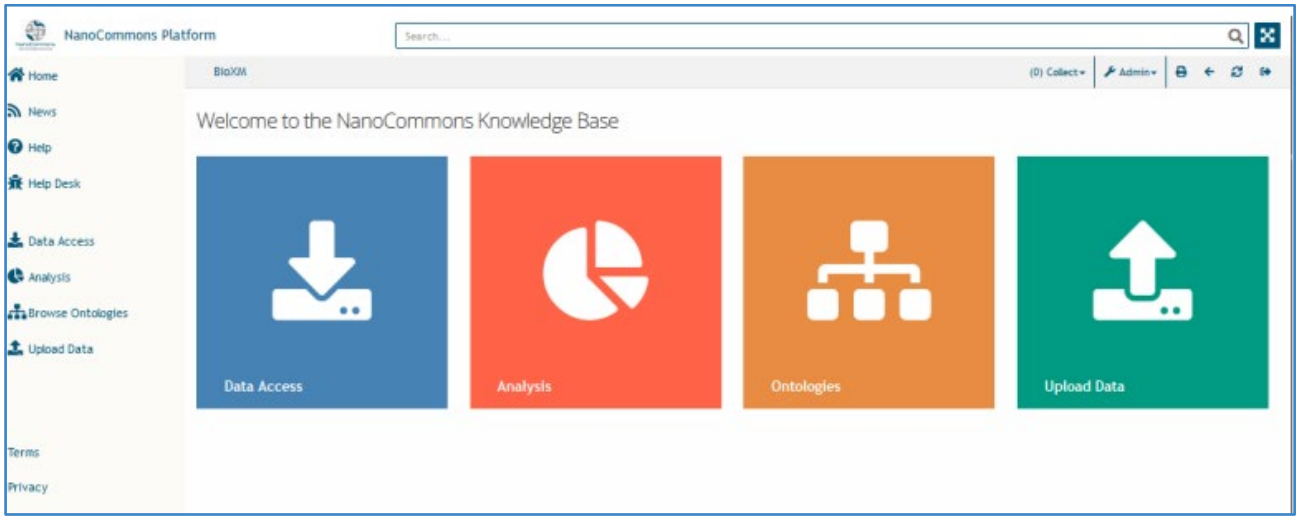


Figure 9. NanoCommons Knowledge Base illustrating the major areas of data upload, data access, data analysis and ontologies to support annotation and integration of data and database schema.

2. NanoCommons User Guidance Handbook

Within the last 1.5 years of the project, NanoCommons, in its role of data and nanoinformatics shepherd, has created a User Guidance Handbook collecting and organising knowledge and training materials for the two strongly interlinked areas of *data management* for nanomaterials and *nanoinformatics,* as well as areas like *Safe-and-Sustainable-by-Design, Risk Assessment, NanoRisk Governance,* and *Nanofabrication* directly profiting from data, tools and services developed with the project and from its activities supporting and engaging with these arenas. The current table of contents, some example pages and the projects collaborating and providing contents to the Handbook are shown in Figure 10. For more details, please see Deliverable D7.3. Similar to the NanoCommons Knowledge Base, which is integrating data from other sources by linking to the corresponding databases and data warehouses and not duplicating the data, the Handbook is not meant to provide all information, knowhow and training materials on the covered areas, concepts and their implementation in platforms, software tools and services but to be the starting point, i.e. a one-stop entry point, for getting this information. This is achieved by short introductions and then references to resources of other projects, activities, service providers but also political, governmental, standardisation and regulatory bodies providing more details or specific tools and models. The contributing projects are highlighted in the handbook in a special section with short summaries and access links to the partners/projects/platforms/networks' websites. Under coordination of partner 7P9, the Handbook will be further developed, extended and updated by actively searching for relevant new contents and recruiting additional partners to contribute contents directly or references to documents, reports and external webpages from which content could be extracted or linked in. In this way, the handbook will become a virtual representation of the past and current nanosafety and advanced materials safety and sustainability research and regulatory landscape in Europe and beyond.

Figure 10. Highlights of the User Guidance Handbook, indicating its table of contents, contributing partners and examples of summaries of key areas and links to training materials and other resources.

3. NanoCommons tools/services

All individual tools and services that have been developed by NanoCommons partners, including the contact points and specialised material can be found in the NanoCommons Service Catalogue.

Examples of the tools and services often requested in TA projects and focus of NanoCommons sustainability efforts are:

- Data management and workflows (e.g., NanoCommons SciNote instance, instance map tool, NanoCommons Knowledge Base,
- Model development, hosting and sharing (e.g., Jaqpot, Enalos Cloud Platform & Isalos Analytics Platform)
- Generation of workflows (e.g., NanoCommons and Enalos NanoCommons KNIME nodes)
- Flexible combination of (internal and external) tools, e.g. the NanoCommons Risk Assessment tool that integrates GUIDENano exposure scenarios, a PBPK model from Jaqpot to get the internal dose and generates a risk prediction based on Points of Departure computed using a gene expression analysis workflow via Enalos Cloud Platform.
- Image Analysis (nanoXtract & nanoimage image analysis tools) as stand alone tools or integrated into the NanoCommons Knowledge Base
- Hosting of curated data in a ready for modelling format (nanoPharos database)
- Protein corona prediction model (stand alone model[18] and integrated into the NanoCommons

[18] D. Power, *et al.* A multiscale model of protein adsorption on a nanoparticle surface. Model. Simul. Mater. Sci. Eng., 27 (8) (2019), Article 084003. https://doi.org/10.1088/1361-651X/ab3b6e

Knowledge Base) and a nanoinformatics protein corona model hosted at the NanoCommons instance of Enalos Cloud Platform

- NInChI calculator (alpha version) and Python code (Jupyter notebook).

While most of these services were specifically developed within NanoCommons, the overarching goal of building a community infrastructure included the integration of existing models and tools, their harmonisation with respect to accessibility as web services or via application interfaces, generation of new ways of access (like via NanoCommons KNIME nodes, Enalos Cloud or Jaqpot model deployments), and the combination into complex workflows like the risk assessment workflow (see Deliverables D6.3 and D6.4). These initial examples of the integration of external resources and tools provided the basis for bringing in more and more tools, services and even full platforms to generate the one infrastructure to provide all available solutions and build new ones by putting the individual pieces together in innovative new ways. Additionally, these services are now being ported and deployed onto computer and cloud resources of the EGI-ACE project[19] and, in this way, are becoming part of the European Open Science Cloud (EOSC) universe and service offerings, guaranteeing even larger visibility, accessibility and long-term sustainability. Partner EwC and the service providers NTUA, NovaM and UM will continue to coordinate these efforts and extend them to services provided by ongoing projects such as NanoSolveIT, SbD4Nano, RiskGONE, CompSafeNano and the outcome of the governance projects, the NanoHouse, and forthcoming Horizon Europe projects.

4. NanoCommons training materials

NanoCommons has organised many workshops/webinars/hackathons during the 4.5 years of the project within the 4 main pillars of activities: (i) Experimental Workflows Design & Implementation, (ii) Data Processing & Analysis, (iii) Data Visualisation & Predictive Toxicity, and (iv) Data Storage & Online Accessibility. It is important to note here that these training activities were always organised jointly with the EU NanoSafety Cluster (NSC) and very often with other EU projects. In this way, and fostered by the fact that Martin Himly (from partner PLUS) was and is chairing NSC WG A Communication, Training and Education. NanoCommons established itself as a major provider, organisator and role model for harmonising the training across all nanosafety projects and in identifying further needs supporting all levels of expertise from basic introductions for early researchers to highly advanced topics for specialists. NanoCommons also functioned as an ambassador to neighbouring communities, like the life science community, by sharing information on training on the ELIXIR TeSS platform. See deliverable D8.3 for more information.

All training materials generated can be found in the NanoCommons Library (with 80 materials), as well as in the NanoCommons YouTube Channel (44 recordings), the NanoCommons Community in Zenodo (with 90 uploads: publications, posters, presentations, lessons, datasets, software, deliverables, newsletters, etc.) and in the NanoCommons community in TeSS, ELIXIR's training platform (with 17 events and 7 materials). All these collections will be kept open in the future to add relevant new training materials and as background materials for upcoming events like the future Venice training schools. Additionally, they are and will stay as a major source of information to be presented in a structured way on knowledge and community platforms like the NanoCommons User Guidance Handbook (see above). Updating of training materials and their interlinking into the User Guidance Handbook will continue to be organised and sustained by partner PLUS (in collaboration with partner 7P9 for the handbook updating).

[19] EGI-ACE project: https://www.egi.eu/project/egi-ace/

Business model for short/long term sustainability

In D10.4 we presented an initial business model for NanoCommons. This plan, proposed to achieve long-term economic sustainability for a NanoCommons Organisation by being in charge of the key elements of the NanoCommons Knowledge Infrastructure: the NanoCommons Knowledge Base, as well as its Consultancy and Services (see Figure 11). In D10.5 and above, we reviewed the feasibility of the presented business model based on the critical evaluation of the TAs, the demonstration cases, and the four main sustainability areas[20] and associated tools (prioritised for short- and long-term sustainability). This was based on the current and estimated future budget needs for running the services and sustaining them not in isolation but integrated into the network of strategic partnerships and the broader (nano)materials and (nano)safety infrastructure landscape (see Deliverables D2.7, D9.3, D10.4 and above).

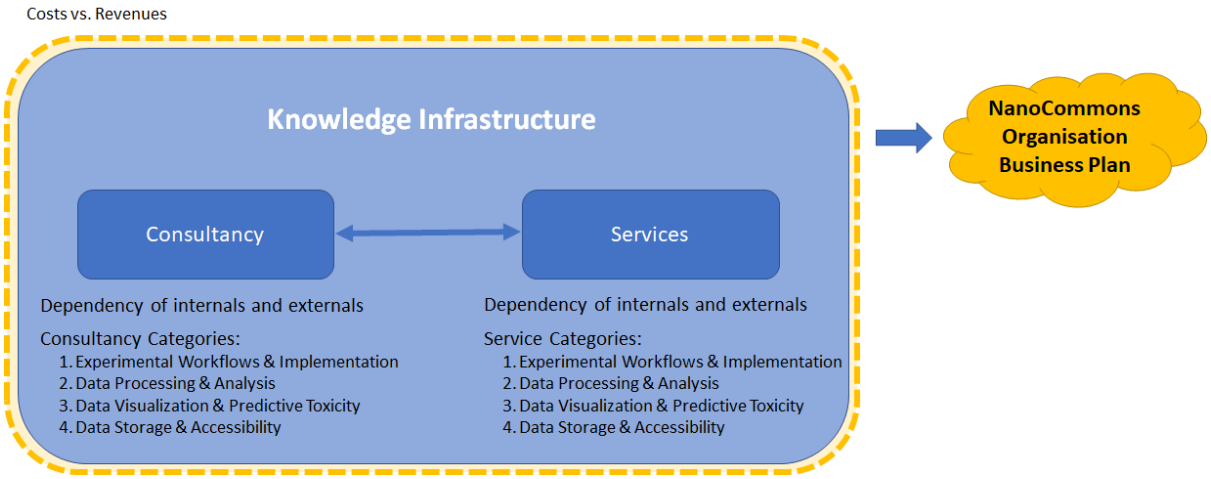


Figure 11. NanoCommons Business Concept as proposed in Deliverable D10.4.

While major steps towards such a commercialisation were achieved during the runtime of the project, the cost estimates for keeping the main services running are still correct and the expected revenues reasonable, the operational basis and fully commercialised services generated by NanoCommons, as a starting community, are limited and do, in our opinion, currently not justify the large overhead of founding this independent organisation. This is especially the case, since the major benefits coming from NanoCommons and the highest impacts are seen and expected in the future as coming from the work on disruptive concepts addressing major challenges, which have the potential to dramatically change the way data is managed and, therefore, address major challenges seen today (see section on the demonstration cases and partly on the TA projects above and in Deliverable 10.5). These concepts have now to be taken over by the community, transitioning it into an advanced community with corresponding tools and services.

As already stressed in the previous testing and evaluation of the sustainability plan (Deliverable D10.5), activities towards sustainability of NanoCommons are now seen as a very important and integrated part of the materials infrastructure ecosystem and are following two parallel tracks:

1. Due to its leading role of creating a network of strategic partners (network of networks), NanoCommons has achieved that its solutions are now adopted by many different projects and activities and are continuing to be developed in these projects. Further uptake by new projects is

[20] Main sustainability areas: NanoCommons Knowledge Base, NanoCommons User Guidance Handbook, NanoCommons tools/services, and NanoCommons training materials

expected and will guarantee continuation in the future. However, and even more importantly, the disruptive concepts prototyped by NanoCommons have become a central part of the (updated) EU-US Nanoinformatics roadmap, led by the EU NSC, the nanofabrication roadmap developed by the NanoFabNet and SusNanoFab projects, and the SSbD-related roadmaps (update on Chemical Strategy for Sustainability/CSS, ETP-SusChem-Roadmap, etc.), which already secured uptake and continuation of the development via national initiatives and should finally lead to integration into the next ESFRI roadmap, planned for 2024/2025.

2. Besides the anticipated public funding described in point 1, possibilities for advanced business models for the parallel commercial exploitation are evaluated with the strategic partners. These are not meant to just add a new player, the NanoCommons Organisation with its limited offerings, to the existing ecosystem, but to create a new way to provide services in a collaborative way, *the commons concept*, which can address much more complex questions by combining functionality. Currently considered options are briefly presented now.

The European Materials Modelling Council (EMMC) published a white paper on "Business Models and Sustainability for Materials Modelling Software"[21]. Since the challenges in this community are very similar to what we see in the nanosafety field and especially for sustaining the NanoCommons outcomes, this white paper was used as a guidance for the business planning and the discussions with the strategic partners. Figure 12 reproduces a part of this report highlighting the importance of online platforms and digital marketplaces, two concepts fully endorsed and fostered by NanoCommons, leading to Software-as-a-Service or even Materials-as-a-Service implementations.

7. Emerging Business Models: Online platforms and Marketplaces

Despite remaining concerns about 'online' and/or cloud-based systems (see Section 6.4.6), there is an overwhelming trend for software to be deployed and used in cloud-based rather than installed systems as any industry report in this area testifies. Key reasons include:

- It costs less compared to legacy systems
- It cuts operational costs
- It enables companies to maintain a consistent working process
- It enables collaboration in large and decentralized teams
- It saves the time needed for setup and training
- It facilitates access to data
- It is devices independent
- It becomes easier to connect applications with each other
- It reduces (or eliminates) the burden of upgrading, maintenance, and safeguarding data

Likewise, digital marketplaces have been growing rapidly as platforms improving ease of purchasing as well as providing marketing and sales channels for the providers of goods and services. Consumer-oriented (B2C) marketplaces have experienced tremendous growth and many industry reports now analyse and predict an even bigger economy for Business-to-business (B2B) digital marketplaces. Key drivers include improved usability and customisation due to machine learning, the scale, speed and security features of latest cloud platforms.

Figure 12. Emerging business models as promoted in the white paper "Business Models and Sustainability for Materials Modelling Software" published by the EMMC[22].

[21] White paper on "Business Models and Sustainability for Materials Modelling Software" : https://emmc.info/wp-content/uploads/2019/01/EMMC-CSA-D5.5_M22_vfinal2-PU-WEBa.pdf

[22] See Footnote 6.

The EMMC then also lists a number of possible business models, which can be used to become part of the ecosystem of online platforms and marketplaces, which are listed below. More details can be found in the white paper[23]. Even if these are not relevant for NanoCommons for the reasons given above, we still list here **single-player models** for completeness.

- Defensive One–Stop Shop Provider
    - Offers complementary products and services in a Marketplace to build a wide portfolio beyond the initial offering.
    - Leverages the client franchise and aims at increasing value per client by answering needs even outside of the legacy positioning.
- Distribution Channel Extension
    - The aim of this strategy is to develop new and complementary distribution channels via the marketplace without jeopardising relationships with existing distributors and legacy channels
- Business Model Transformation
    - Players developing this strategy usually see their business at risk either because of upstream or downstream disintermediation or due to strong changes in their ecosystem, such as clients and suppliers going from captive to competitive.

More relevant are the **multi-stakeholder models** since they manifest the collaborative approach.

- Product community
    - helps to build a community around products
    - especially relevant to digital goods
    - primarily creates value to sellers and buyers by creating an active community of like-minded people
    - firms provide social network functions and focus their key activity on community building
    - commission fees are the dominant revenue form
- Offline services on-demand
    - match service firms with consumers
    - exchanged services are delivered offline and therefore require some form of scheduling
    - None of the marketplaces creates significant value through the platform community. Rather, these firms focus their activities on generating solutions to increase efficiency. The companies in the cluster generate revenues through commissions from the sellers, while buyers mostly use the marketplace for free.
- Online services
    - Companies in this cluster share the characteristic that they offer services that are delivered via the internet.
    - This includes services that involve individuals ‘sharing’ their previously untapped skills.
    - The cluster also includes firms that aggregate professional freelancers such as scientific researchers.
    - Marketplace participation provides sellers with a clear advantage in reaching target audience
    - In many cases, demand-side users receive value from the community around the core service
    - The fee is mostly charged as commission or subscription

[23] See Footnote 6.

However, one key issue has to be solved for all such models: as long as they are based on rigid contracts for linear deliverables, e.g., contracts only between two specific partners, every actor (consortia but also single project partners or commercial entities, funding bodies and private investors, research as well as supply infrastructures,...) is playing their own game trying to optimise their own benefit as much as possible (see Figure 13).

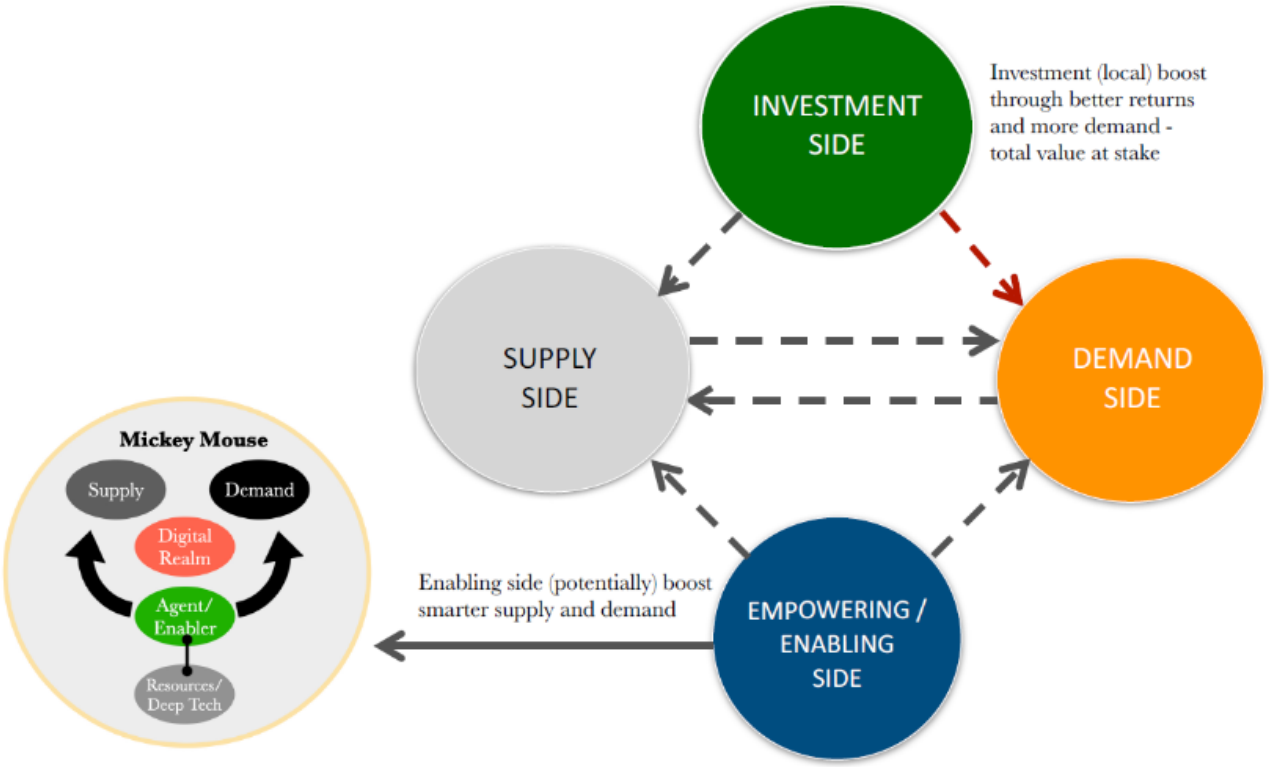


Figure 13. Actors relevant for a multi-stakeholder business model with their (rigid) contracts representing their individual business interests.

Instead, the multi-stakeholder model could be built following the concept of separation of powers, this also being the basis of modern democracies. Figure 14 shows one possible structure for implementing the concept, where there is not one single omnipotent body defining the rules of the marketplace, but a set of governmental institutions, appointed by all stakeholders in the ecosystem and performing checks and balances on each other. The exact setup of these institutions and the general rules of conduct still need to be specified and agreed on, but early, still theoretical implementations show the immense societal impact such ecosystems might have. Technical solutions like BlockChain and cryptocurrencies are already being explored as the basis for the daily business, which guarantee that transactions are secure and traceable but with the additional advantage that data could be used as the main currency, directly acknowledging the value of it, and real money only has to come into the play, if stakeholders, e.g., large industry, want to profit from services or data without providing services themselves.

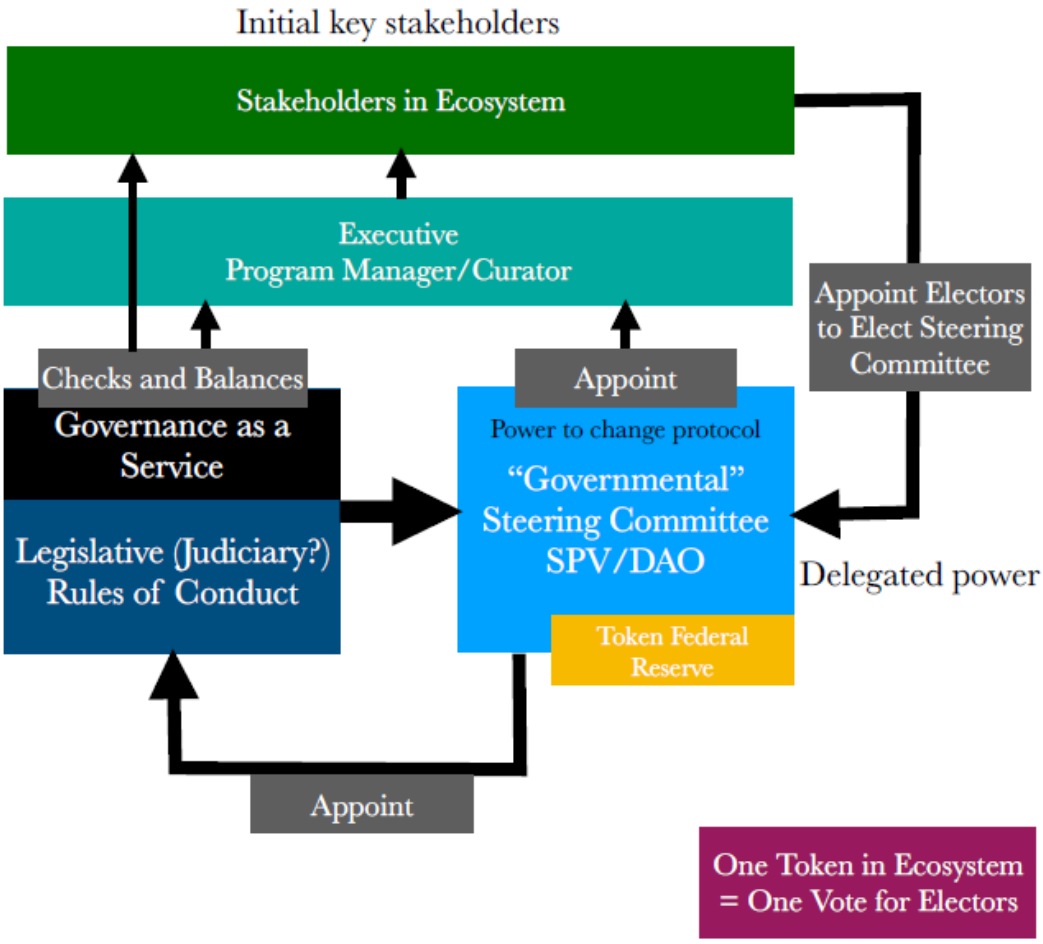


Figure 14. Separation of powers as underlying governance concept for a multi-stakeholder business model[24]where suppliers trade or exchange services collectively based on tokens with a specified value, and only need to pay for services if they are themselves not also providing services to the community.

[24] Private communications by Mats Brodén, Embedded Nano Europe AB, Stockholm, Sweden, www.embeddednano.com

Conclusion

The work carried out by NanoCommons during the project lifetime has allowed us to establish NanoCommons as a starting community infrastructure. As clear benefits of the central infrastructure have already been recognised by its users, individual groups, institutions and large projects, and the provided concepts and services have the potential to change the way data is managed and reused to address major actual challenges, the NanoCommons community will continue to be developed, expanded to more and more areas related to nanosafety and beyond, and, in this way, become an advanced community, contributing and being used and fed by all interested stakeholders.

The ideas, concepts, integrated workflows combining the benefits of *in chemico*, *in vitro* and *in silico* experiments, and and their realisation as NanoCommons services spanning the four sustainability areas (NanoCommons Knowledge Base, NanoCommons User Guidance Handbook, NanoCommons tools/services, and NanoCommons training materials) will live on as part of different RIA projects or services provided by individual NanoCommons partners or small groups or Consortia (and associated) partners. However, further large-scale developments of the NanoCommons Infrastructure as a single platform and integration of more and more services essential for addressing the increasingly complex challenges of the (nano)materials and (nano)safety communities can only be achieved in a coordinated and consolidated effort of all stakeholders. These include not only members from the mentioned communities but also from all the neighbouring areas that need to be integrated fully in order to achieve the Safe-and-Sustainable-by-Design and circular economy goals. Additional public funding will be needed, which is to a very limited amount already secured by the involvement of NanoCommons partners in the EGI-ACE and WorldFAIR projects tasks with by adding new (NanoCommons) services to the EOSC and improving the interoperability within and between communities, respectively. Even if these help to integrate the NanoCommons results even deeper into the European infrastructure landscape, additional seed funding needs to come, in the best case scenario, by being listed on the ESFRI roadmap. In parallel, the commons concept should be extended to include the possibility to offer commercial services not limited to the current rigid structures of bilateral negotiations but as part of a multi-stakeholder business model defining clear rules of engagement. Such a system would not only benefit the directly involved parties of a transaction but the community and the society as a whole, by increasing the availability of knowledge and data.

The NanoCommons consortium are fully committed to working together with our strategic partners to lead the way towards this central research and innovation infrastructure, since we regard it as the only way to address the current challenges of reaching a more sustainable and circular economy that protects human health and the environment as expressed in the UN SDGs, the European Green Deal, the EU Chemicals Strategy for Sustainability, and similar action plans world-wide. Besides the technical challenges, however, we still see the need for a number of necessary attitudinal changes regarding the need for, and value of FAIR and Open data, especially to SMEs whose time and resources for data management are limited.

Firstly, as with infrastructures for our daily life, research infrastructures are seen as something that is important, but that needs to be provided by some central, not clearly defined entity (e.g., the state) and, in the best case, free of charge. This becomes obvious in some of the statements given in many of the TA evaluations. We agree with this statement when it comes to the central data infrastructure, since allowing the sharing and reusing of data produced with support of public funding should not be limited by commercial

considerations. Otherwise, the innovative potential would be extremely reduced and only available to players able to afford buying data or reproducing it. However, other services, such as those in the nanoinformatics and data-consultancy field, need continuous maintenance and development to keep up with the state-of-the-art, which requires stable funding. Therefore, we believe that domain-specific infrastructure building needs to be considered by all stakeholders as a community effort, where all performed research is aligned with the existing infrastructure as a basis for sustainability and enhanced visibility and demand. Use of infrastructure services and integration of new services to complement the existing ones should be budgeted into every new research project. This should be complemented by specific funding for the infrastructure itself for building and maintaining the core services like data sharing and integration services and partly also sustaining specific services, which cannot be maintained by the original developer anymore.

Secondly, research often continues to be regarded as too early in the innovative process to be relevant for supporting the collective effort to reach the UN SDGs; this results in the misconception that the establishment of an infrastructure with its potential of effectively and efficiently supporting the SGDs is also irrelevant. To change this, NanoCommons considered raising awareness of the importance of the SDGs as one of its major goals and implemented evaluations of all its results according to the SDGs in question; NanoCommons was one of the first nanosafety projects to have implemented this quality-monitoring process, and are currently finalising the process and findings into a publication to support the community further in demonstrating the value inherent in FAIR and Open nanosafety data, tools and models to support the SDGs. We hope that this process will be increasingly adopted by ongoing and future projects as a best-practice approach. Through this, we envisage that social, environmental, and economic sustainability goals could become more generally accepted and adopted as quality measures of publicly funded research, to ultimately define tangible scientific success criteria, similar to the number of publications and other dissemination actions.

ANNEX 1 – NanoCommons Brand Guideline