Electronic Supplementary Material (ESI) for RSC Sustainability.

Supporting Information

The role of FAIR nanosafety data and nanoinformatics in achieving the UN Sustainable Development Goals: the NanoCommons experience

Beatriz Alfaro Serrano[1], L. Cristiana Gheorghe[2], Thomas E. Exner[3], Susanne Resch[1], Clemens Wolf[1], Martin Himly[4], Andreas Falk[1], Nathan Bossa[5ʃ], Socorro Vazquez[5], Anastasios G. Papadiamantis[2,6,7], Antreas Afantitis[6,7], Georgia Melagraki[8], Dieter Maier[9], Haralabos Saramveis[10], Egon Willighagen[11], Vladimir Lobaskin[12], Jonathan D. Oldfield[2], Iseult Lynch[2,7*]

File contains:

1. Questionnaire used to evaluate the Transnational Access provision from NanoCommons
2. Completed Transnational Access projects
3. Final set of SDGs identified by the NanoCommoms TA providers and users
4. Searchable version of Table 1 from the main manuscript.

Supporting Material 1 - TA evaluation questionnaire template

Evaluation Template for NanoCommons TAs

The aim of this document is to help us to evaluate the applicant's experience and satisfaction with the delivery and outcomes of their TA, to help us continuously improve. Furthermore, the services currently offered as TAs need to be sustained in the future, potentially as pay-to-use services offered by the NanoCommons Knowledge Infrastructure (KI) - to that end, we are interested to understand if and what you might be willing to pay for such services. This questionnaire will thus help us to optimise the benefits generated by the KI for users as well as service providers.

NanoCommons TA providers together with the TA applicant are requested to complete this document.

→ Questionnaire A – To be filled-in by the NanoCommons TA provider(s):

1. TA application number: xxx
2. Name of TA applicant: xxx
3. Surname of TA applicant: xxx
4. Affiliation of the TA applicant: xxx
5. Main contact from NanoCommons for the TA (NanoCommons TA provider) – Name: xxx
6. Affiliation of the NanoCommons TA provider: xxx
7. Other NanoCommons partners involved:
   ☐ Yes → Which other NanoCommons partners are involved? *(Enter the name of the organizations in text form)*: xxx
   ☐ No
8. Kind of category of the provided service/TA:
   ☐ Experimental Workflows Design & Implementation
   ☐ Data Processing & Analysis
   ☐ Data Visualisation & Predictive Toxicity
   ☐ Data Storage & Online Accessibility
9. Discipline of the service/TA: (*Example: Safe-by-Design, In silico modelling, Data and metadata curation, …)*

- xxx

10. Time expected vs. real time needed for the TA:

	Lead partner	Partner 2	Partner 3	etc.
Expected time (in months):				
Real time (in months):				

11. Reporting / publication of the awarded TA (including grey literature or publication on the NanoCommons Webpage):
    ☐ Yes → Reference: xxx
    ☐ No

12. Estimation of costs for this TA:

	Lead partner	Partner 2	Partner 3	etc.
Direct personnel costs (& related PMs)				
Direct costs of subcontracting (& related PMs) (if applicable)				
Other direct costs (Travel, Equipment, Other goods and services…)				
Based on the total cost, what % add-on for the Coordination / promotion etc. by NanoCommons would be appropriate? (*e.g.* 2%, 5%, 10%, 20%, 25%)				

13. Has the TA provider (NanoCommons TA expert) been involved in similar TAs?
    ☐ Yes → Which one(s) (TA number)?: xxx
    ☐ No

14. If YES in the previous question, would it be possible to make a guideline to standardise at least a part of the TA so potential TA applicants would be able to implement a part of the TA on their own or with minimal guidance by the experts or to get started based on the training material?
    ☐ Yes → Re-estimation of costs: xxx
    ☐ No

15. From your experience with this and similar TAs and other dissemination activities, how would you describe the commercial potential and the market for the used services? *(Enter your answer in text form)*

16. How relevant do you see the services for the commercial sustainability of NanoCommons? (*Select just one option*)
    ☐ Very
    ☐ Slightly
    ☐ Neutral
    ☐ Slightly not
    ☐ Not at all

17. How relevant do you see the NanoCommons Knowledge Infrastructure for the sustainability of the service/TA? (*Select just one option*)
    ☐ Very
    ☐ Slightly
    ☐ Neutral
    ☐ Slightly not
    ☐ Not at all

18. Were any *social* sustainability goals addressed directly or indirectly *(e.g. through data accessibility for re-use – see here for ways artificial intelligence supports the SDGs)* by the TA? If **YES**:
    - Which SDGs have been addressed? (*More than one is possible*)
        ☐ SDG 3: Good Health and Well-Being → If YES, why?
        ☐ SDG 5: Gender Equality → If YES, why?
        ☐ SDG 6: Clean water and Sanitation → If YES, why?
        ☐ SDG 8: Decent work and Economic Growth → If YES, why?
        ☐ SDG 10: Reduced Inequalities → If YES, why?
        ☐ SDG 11: Sustainable Cities and Communities → If YES, why?
        ☐ SDG 16: Peace, Justice and Strong Institutions → If YES, why?
        ☐ SDG 17: Partnerships → If YES, why?

    - How might the services help NanoCommons to support the achievement of these goals on a more global scale? *(Enter your answer in text form)*

19. Were any *environmental* sustainability goals addressed, directly or indirectly, by the TA? If **YES**:
    - Which SDGs have been addressed? (*More than one is possible*)
        ☐ SDG 6: Clean water and Sanitation → If YES, why?
        ☐ SDG 11: Sustainable Cities and Communities → If YES, why?
        ☐ SDG 12: Responsible Consumption and production → If YES, why?

☐ SDG 13: Climate action → If YES, why?
☐ SDG 14: Life below water → If YES, why?
☐ SDG 15: Life on Land → If YES, why?
☐ SDG 17: Partnerships → If YES, why?

- How might the services help NanoCommons to support the achievement of these goals on a more global scale? *(Enter your answer in text form)*

20. Were any *economic* sustainability goals addressed, directly or indirectly, by the TA? If **YES**:
    - Which SDGs have been addressed? *(More than one is possible)*
      ☐ SDG 8: Decent work and Economic Growth → If YES, why?
      ☐ SDG 9: Industry Innovation and infrastructure → If YES, why?
      ☐ SDG 12: Responsible Consumption and production → If YES, why?
      ☐ SDG 17: Partnerships → If YES, why?
    - How might the services help NanoCommons to support the achievement of these goals on a more global scale? *(Enter your answer in text form)*

21. If you were not able to answer the last 3 questions about the *social, environmental and economic* sustainability goals that have been addressed by the TA, would you be interested in participating in an online training on how research can support the SDGs?
    ☐ Yes
    ☐ No

22. If you answered YES to the last question, would you be willing to pay for the offered training on utilising your research in support of the SDGs?
    ☐ Yes → Enter your contact details here (Name, Affiliation, Email address): xxx
    ☐ No

→ Questionnaire B – To be filled-in by the TA applicant:

1. Need of the TA applicant before applying for the TA: xxx

2. Expected value to the TA applicant / Benefit of the TA for the applicant (BEFORE the TA was in place):
    - New tool to further my research (*e.g.* would have taken a PhD student 2+ years to develop)
    - Would not have been possible to do the research at all
    - Other: xxx *(enter your own)*

3. Experienced value of the TA outcomes (Applicant Satisfaction) (AFTER the TA was finished)
    - Has facilitated me to leverage new grant - valued at … €
    - Has facilitated high impact publication - valued at …€
    - The model would have taken a postdoc X months to develop - valued at …€
    - Hiring a data manager would be …€ / year
    - Other: xxx *(Enter your own)*

4. Reporting / publication of the TA outcomes (by the TA applicant):
   ☐ Yes → Reference: xxx
   ☐ No

5. Expected = Received Benefit [%] (TA applicant's opinion) (*Select just one option*)
   ☐ Fully
   ☐ Partially
   ☐ Not at all

6. Consider now the additional value created for you from the TA you experienced. Based on the actual cost of providing the TA to you, as estimated by the NanoCommons partner(s) involved (question 12 of the previous section), would you consider requesting the service within a commercial setting? If yes, would this price be accepted by the TA applicant? (Pricing adapted to the service/tool being analysed and the associated infrastructure and personal costs involved in the delivery of the service)
    - xx € *(see question 12 of the previous section)*
      ☐ Yes
      ☐ No → Why?
      How much would you be willing to pay?: xxx €

7. Independent of the answer you gave to the question above on commercial profitability, the service might provide you or society with other benefits in terms of sustainability. Such benefits might enable cross-financing from other sources (*e.g.* other revenues, public investment or public-private partnerships, etc.). Which benefits

do you see and how do they support reaching the UN Sustainable Development Goals (SDGs)?

☐ No, I do not see the benefits.
☐ Yes, I do see further benefits:

- Which SDGs have been tackled by this TA? *(More than one is possible)*
    - ☐ SDG 3: Good Health and Well-Being → If YES, why?
    - ☐ SDG 5: Gender Equality → If YES, why?
    - ☐ SDG 6: Clean water and Sanitation → If YES, why?
    - ☐ SDG 8: Decent work and Economic Growth → If YES, why?
    - ☐ SDG 9: Industry Innovation and Infrastructure → If YES, why?
    - ☐ SDG 10: Reduced Inequalities → If YES, why?
    - ☐ SDG 11: Sustainable Cities and Communities → If YES, why?
    - ☐ SDG 12: Responsible Consumption and production → If YES, why?
    - ☐ SDG 13: Climate action → If YES, why?
    - ☐ SDG 14: Life below water → If YES, why?
    - ☐ SDG 15: Life on Land → If YES, why?
    - ☐ SDG 16: Peace, Justice and Strong Institutions → If YES, why?
    - ☐ SDG 17: Partnerships → If YES, why?

- What is the specific benefit you see there, for each one of the selected SDGs above? *(Enter your answer in text form)*

Supporting Material 2 - Completed Transnational Access projects

List of the completed Transnational Access (TA) projects, and the TA provider(s) and TA users:

TA project number and short name	TA Provider	TA user
NC01 -Ontologies for nanodescriptors generated by molecular modelling	Maastricht University	Stockholm University, Sweden
NC02- Ontology annotation of nanomaterial safety data to support semantic data integration and analysis	Maastricht University	University of Plovdiv, Bulgaria
NC03 - Data curation and harmonization: increasing fairness scores and availability of data generated under EU projects	University of Birmingham	University of Aveiro, Portugal
NC04 - Computational analysis of mesothelioma expression profiling data with Enalos Informatics Tool	NovaMechanics Ltd.	University of Eastern Piedmont, Italy
NC05 - Extraction of image descriptors from TEM microscopy images	NovaMechanics Ltd.	University of Burgos, Spain
NC06 - Creation of a web implementation of a PBPK model on polyethylene glycol-coated polyacrylamide (PAA-peg) nanoparticles on rat	National Technical University of Athens	University of Nevada Reno, USA
NC07 - Nanoparticle's zeta potential prediction using image nanodescriptors	NovaMechanics Ltd.	University of Burgos, Spain
NC08 -SmartNanoTox - Data management and curation	University of Birmingham	Université de Lorraine, France
NC09 - Data curation of exposure experiment: increase the dat availability from the nanoFASE project	University of Birmingham	LEITAT Technological centre, Spain
NC10 - Structural alterations of allergen upon nanoparticle binding	University College Dublin	Paris Lodron University of Salzburg, Austria
NC11 - Nanoparticles as adjuvants for AIT: impact on antigen processing and presentation	University of Birmingham	Paris Lodron University of Salzburg, Austria
NC12 - Cremations, Urns and Mobility (CRUMBEL). Ancient population dynamics in Belgium, XRD analysis and crystallographic modelling	University of Birmingham	Vrije Universiteit Brussel, Belgium
NC13 - Computational implementation of a validated cell cytotoxicity classifier for metal oxide nanoparticles and integration into NanoCommons infrastructure	National Technical University of Athens	Institute of science and technology for ceramics (ISSMC), Italy

NC14 - Ontological annotation, data enrichment, annotation and curation of functionalized nanoparticles used in cancer treatment (EvoNano)	University of Birmingham	University of Novi Sad, Serbia
NC15 - To assist the Diamond SARS-CoV-2 Mpro fragment screening program in selecting compounds for further analysis based on predictive metabolism and toxicology	National Technical University of Athen & NovaMechanics	Informatics Matters, UK
NC16 -Data capturing, storage and management of high quality, curated and harmonized data generated under the ASINA project while increasing fairness scores	University of Birmingham	Transgero Limited< Ireland
NC17 - Mixture (nano)toxicity in the Daphnia magna Model	University of Birmingham	Brazilian Nanotechnology National Laboratory, Brazil
NC18 - Measure size and features of nanoparticles in an automated way (using NanoImage)	National Technical University of Athen	National Centre For Scientific Research Demokritos, Greece
NC19 - Measure size and features of nanoparticles in an automated way (using NanoXtract)	NovaMechanics Ltd.	National Centre For Scientific Research Demokritos, Greece
NC20 - Predictive toxicity assessment of semiconductor quantum dots that are used as fluorescence probes – adverse effects on the human lung epithelial carcinoma cell line A549 ("QD-cytotox")	NovaMechanics Ltd.	University of Natural Resources and Life Sciences, Vienna, Austria
NC21 - Implementation and validation of the FAIR principle for data produced in SAbyNA project to ensure that high quality data is flowing in data repository (NanoCommons warehouse)	University of Birmingham	LEITAT Technological centre, Spain
NC22 - Nanosafety data from FAIR Data Austria institutions – Part 1	Seven Past Nine / University of Birmingham	University of Vienna, Austria
NC23 - PBPK model on 99m-Technetium-labelled carbon nanoparticles inhaled by humans: Implementation in R and integration into the NanoCommons modelling toolbox	National Technical University of Athens	National Institute for Industrial Environment and Risks, France
NC24 - Aligning the NanoCommons KnowledgeBase functionality with IUCLID6 and EUON's data needs	Biomax / University of Birmingham	EUON, Finland
NC25 - Stochastic optimisation for grouping nanoPBPK model parameters and and estimating their values: New methodology and service development	National Technical University of Athens	University of Nevada Reno, USA

NC26 - Development, validation and web implementations of environmental nanoQSAR models	National Technical University of Athens	US Environmental Protection Agency, USA
NC27 - Nanosafety data from FAIR Data Austria institutions – Part 2	Seven Past Nine / Biomax	Technical University Graz, Austria
NC28 - Integration and standardization of real-time OF2i data and its applicable/close regulatory field	Seven Past Nine	Brave Analytics Ltd.
NC29 - Data integration for online analysis of production parameters on material properties & quality	Seven Past Nine	TEMASOL, Switzerland
NC30 - Bioinformatics analysis of the transcriptomics TIO2 dataset	University College Dublin	National Research Centre for the Working Environment, Denmark
NC31 - In silico characterisation and a QSAR model for in vivo lung inflammation for set of 50 SmartNanoTox materials	NovaMechanics Ltd., University of Birmingham	Helmholtz Zentrum München, Germany

Supporting Material 3: Final set of SDGs identified by the NanoCommoms TA providers and users

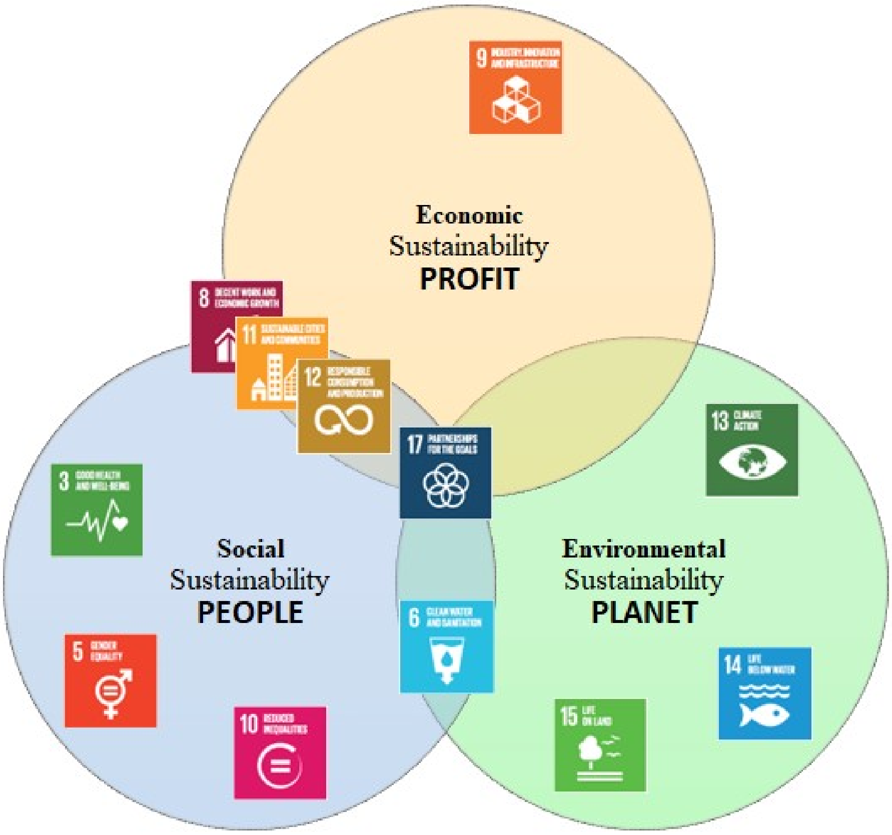

Figure S1. Representation of the SDGs identified as being addressed in the different NanoCommons TA projects (from the TA applicant and TA provider perspective) following the Training provided within NanoCommons on the SDGs and the wider discussions on the value of FAIR nanoEHS data and nanoinformatics tools and approaches.

Supporting Material 4: Searchable version of Table 1 from the main manuscript

Applications of Nanotechnology	NanoCommons TA project: role of FAIR nanoEHS data and/or nanoinformatics in supporting the SDGs	How nanoinformatics data and/or tools directly or indirectly support the SDGs (not a 1:1 mapping but rather an overview for each of the goals)
Energy storage, production, and conversion	NC01 - Ontologies for nanodescriptors generated by molecular modelling ● Inorganic NMs such as metal oxides are key to energy storage and capture devices. ● Ontology terms covered materials descriptors as well as materials application areas and meta-models that bridge across scales. ● Documentation of the interlinkages between materials models via MODA templates to link models for materials properties with models for materials functionality (e.g., energy capture). NC12 - Cremations, Urns and Mobility. Ancient population dynamics in Belgium, XRD analysis and crystallographic modelling ● Mapping historical cremated bones: use of spectral data to understand historical burial practices ● Links to social and cultural norms in different countries related to burial practices and energy demands associated with these. ● Ethics of data-re-use and data governance.	SDG7: Affordable & clean energy - The *in silico* data enrichment tools can help to identify NMs features optimised for energy capture/storage, that support reduced greenhouse gas emissions (e.g., through more complete combustion) and/or for use in construction materials, driving sustainable and green innovation. - Full documentation of models (via MODA) is a critical step in driving uptake / market acceptance of the tools (i.e., standardisation) and the detailed tutorials and user guidance are key steps in democratising access for global south to models and datasets. SDG4: Quality Education - Extensive training materials have been developed to accompany all NanoCommons models, as part of the efforts to democratise access to advanced approaches. Additional materials for use in schools and universities are being developed also, enabled by the fact that all NanoCommons models have free user-friendly graphical user interfaces, requiring only an internet connection rather than specific software licences or other potentially prohibitive resources.
Agricultural productivity enhancement	NC3 - Data curation & harmonization: increasing fairness scores and availability of data generated under EU projects (NanoFASE, NanoFARM) ● Agricultural productivity is dependent on soil quality including	SDG15: Life on land - The impact of intensive agriculture on soil quality has been dramatic with many soils having < 10 years of productivity remaining, which has consequences for food security. The development of streamlined data

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	bacterial richness and earthworm bioturbation to aerate. ● Datasets covered impacts of Ag NMs on earthworms and soil and water mesocosms. ● Development of instance maps to structure the data and associated metadata to facilitate re-use of the data, including for development of predictive models. ● Implementation of new ontology terms and mappings for NMs transformation processes such as sulfidation which determine NMs persistence & ecosystem-level impacts such as soil quality. NC07 - Using image descriptors to predict nanomaterials zeta potential ● Development of agrochemicals: zeta potential can be used to predict the stability and dispersibility of the particles in the formulation. This can affect efficacy and environmental impact of agrochemicals. By manipulating zeta potential of particles, it may be possible to enhance performance and reduce the environmental impact of agrochemicals. ● Zeta potential of soil particles can affect the ability of the soil to retain nutrients and water, as well as the movement of pollutants. Predicting the zeta potential of soil particles can help to optimise management practices such as irrigation, nutrient application, and soil remediation. ● Climate change, gender inequality and responsible production all converge in managing soil quality.	curation processes for soil quality data, and earthworm / bioturbator data (e.g. NanoFASE, NanoFARM, & data regarding the impacts of nanomaterials on soil microbial composition and functioning and earthworm behaviour), provides a strong basis for further harvesting relevant datasets, both to facilitate the development of models to predict impacts of treatments on soil health and thus productivity (and health) and to develop relevant policy interventions to support and drive initiatives to improve soil health, while maintaining productivity and sustaining livelihoods in developing, agriculture-based economies. SDG12: Responsible consumption & production - The TA project with Brazil supported the introduction of FAIR data management approaches to the national centre for nanotechnologies, from which it also rolled into national standardisation activities on nanotechnologies including the MCTI-INMETRO-SisNANO programme. for Certification of Nanoproducts). Early access to the state of the art in nanosafety data management and FAIR data, and the expertise to support its implementation in the Brazilian context has been extremely beneficial, as has the experience of understanding how to adapt technologies and solutions for the local context integrating local knowledge.
Vector and pest detection and control	NC10 - Structural alterations of allergen upon nanoparticle binding & NC17 - Mixture (nano)toxicity in the *Daphnia magna* Model ● Both of these TAs considered the interactions of NMs with co-	SDG16: Peace and Justice through strong institutions - Nanomaterials safety is an example of a community of practitioners who

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	pollutants, and the role of the biomolecule corona directly (allergens) and indirectly (binding co-pollutants and changing their bioavailability) on the activity / toxicity. ● Such approaches / models can also be applied to assessment of the role of NMs as vectors for viruses or bacteria, or to design NMs-based sensors for key proteins or environmental DNA (so-called eDNA) for example. ● Models for mixture assessment are critical to understand the potential risks of NMs activating as vectors for transport of other entities, including bacteria. Indeed, air pollution particle levels were found to correlate with Covid-19 infectiousness. NC16 - Data capturing, storage and management of high quality, curated and harmonized data generated under the ASINA project while increasing fairness scores ● ASINA were one of the first projects to implement the NanoCommons data shepherding approaches, applying them to management of case studies. ● A case study explored anti-microbial and anti-biofilm coatings for textiles, and established reporting guidance and data templates to facilitate researchers and the industrial community to disclose appropriate functionality data via the FAIR principles. ● Datasets were made increasingly FAIR through data shepherding, and SOPs for data management were implemented (19).	tried to pre-empt problems such as unsafe nano-enabled products reaching the market, and public opinion turning against the technology as a whole (as was the case what genetically modified organisms in the EU), through application of governance approaches early. This also involved ongoing engagement with all relevant actors including regulatory agencies and industry to ensure that regulators were aware of scientific progress. That said, there is still room for further improvement - for example, research data is still difficult to integrate into regulatory risk assessments despite the fact that research is usually a decade ahead in understanding than regulation is. Data and model documentation, including rich metadata, is a key aspect to improving the re-use of research data and models in governance, regulatory risk assessment. NanoCommons efforts, including in elucidating the need for a dedicate role of "data shepherd" to support this transition, is key.
Water treatment and remediation	NC17 - Mixture (nano)toxicity in *Daphnia magnal* - Supporting FAIR data practices in Brazil ● Project involved knowledge transfer to support establishment of FAIR data management practices in national Brazilian nanotech	SDG6: Clean water & sanitation - There were an estimated 13.7 million infection-related deaths in 2019. Malaria alone kills half a million annually, despite progress in impregnating nets with pesticides targeting mosquitos. Textile hygiene

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	labs, and then further roll-out to other laboratories in Brazil. ● Implemented Electronic Laboratory Notebook, Instance Maps and data integration in KnowledgeBase for a set of studies exploring the impact of graphene (and its adsorbed biomolecule corona) as a mediator of the toxicity of heavy metal pollution in aquatic systems (27). ● Nanomaterials' capacity to absorb co-pollutants, and the impacts of adsorption to NMs for the toxicity of co-pollutants was explored & all data/ metadata made FAIR. ● Use of the "Instance map" tool allows understanding of impact of the environment and points where the NMs may transform and thus behave differently. NanoCommons has proposed instance maps as a tool for quality assurance and for integration and harmonisation of datasets. ● Extensive training materials developed to support wider roll-out in Brazil. NC29 - Data integration for online analysis of production parameters on material properties & quality ● Continuous or in-line characterisation of materials properties and quality raises additional data management challenges, related to the quantity of data and the need to understand what is relevant for internal Quality control versus what might have intrinsic value for broader nanoEHS assessment and modelling, for example. ● Data shepherding approaches will maximise the transfer of knowledge and data.	and infection control measures have become increasingly important in recent years due to the growing concerns about textiles as fomites (inanimate objects that can carry and spread disease and infectious agents) in healthcare settings (26). NMs composed of silver and copper have antimicrobial properties and are being embedded into textiles for a range of essential (e.g., wound and burn dressings) and less-essential (e.g., odour reduction socks and sports cloths) applications. However, concerns exist that the NMs are quickly washed away thus limiting long-term effectiveness and thus applications of safe-by-design to ensure longevity of effect are essential, but not inadvertently introducing new problems related to over-persistence in the environment and/or at end of life. Sharing of data and experiences, such as via the ASINA case study on antimicrobial textiles, are thus essential to support transfer of knowledge and enable new innovations to support global health and wellbeing and to ensure that the advances are not limited to global north countries, given that the majority of infectious-disease deaths occur in the global south. SDG14: Life below water - Daphnia magna are an important indicator species for water pollution globally, with 2 tests included in the OECD Mutual Acceptance of Data (acute and chronic (reproductive) toxicity to daphnia) framework, meaning that data from one country performed in accordance with the agreed Test Guidelines is accepted for regulatory purposes in another country. Thus, sharing of data from standard (OECD) test guidelines is critical to support regulations globally, and to enable nanomaterials approved in one jurisdiction to be approved elsewhere on the basis of the same datasets.

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Disease diagnosis and screening / Health monitoring	NC15 - Assist the Diamond SARS-CoV-2 Mpro fragment screening program in selecting compounds for further analysis based on predictive metabolism and toxicology ● Covid rapid response demonstrating potential of re-use of both data & modelling tools to address urgent healthcare issues. ● Reduction of inequality (of access and knowledge) through collaboration, knowledge and informatics tool and expertise sharing. ● Workflows for model integration and screening of existing drugs fragments. NC33 - Bioinformatics analysis of transcriptomics TIO_2 dataset (from inhalation exposure studies in the context of the SmartNanoTox project) ● Biomarkers of disease are typically identified from omics data, and identification of molecular initiating events leading to Adverse Outcomes is expected to accelerate understanding of pollution-related disease mechanisms. ● Existing data processing workflows were applied (re-use of tools and approaches) to datasets and the resulting processed data was FAIRified; ● Potential to reduce gender inequality in medicine through considering impact of sex on model results, e.g. modelling male vs female sera. NC4 - Computational analysis of mesothelioma expression profiling data with Enalos Chem/Nano Informatics Tools: potential to support disease diagnosis and screening by identifying significant genes that	SDG10: Reduced inequalities - Agriculture is one of the major polluters due to excessive use of nitrogen-based fertilisers (N_2O is a greenhouse gas), much of which runoff into water bodies, and over-reliance on pesticides. NanoCommons datasets and models enable tuning of nanomaterials properties and prediction of their fate and behaviour and/or toxicity to soil and water environments, providing a basis for design of nano-enabled agrichemicals that are less harmful to soil, air and water whilst delivering the pest control needed. - Democratisation of access to data and models, through provision of user-friendly graphical interfaces with no need for coding, and the underpinning datasets as easily downloaded formatted sheets, is a major step towards reducing inequalities in terms of knowledge and access across boundaries and scales. Nanoinformatics and FAIR nanomaterials and nanosafety data and models provide an initial understanding of the potential hazards and risks of nanoscale materials and a basis from which to tailor existing models to the local needs and conditions of communities in the global south. Use of open access tools and software means that the tools can be easily tailored to local needs by software developers, and where the relevant expertise is not available the contact details for collaborative re-development of models for specific needs are provided with all NanoCommons models and tools. - A key finding from the Covid-related TA project was that once models have been developed it is relatively straightforward and quick to re-purpose them for other applications, and that datasets collected and curated for one purpose can be leveraged and mined to support other, often quite different, research and policy questions. This was a strong argument for FAIR data practices.

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	can discriminate between pathological and healthy samples. ● The developed QSAR model can predict the long-term toxicity of fibre nanomaterials based on gene expression signatures, which can aid in screening and diagnosis of diseases related to nanomaterial exposure. ● The standardization and normalization of expression profiling data can improve data comparability across studies and facilitate the identification of biomarkers of disease. ● The Enalos KNIME nodes used in the workflow can enable the integration and analysis of diverse data types, such as chemical properties and toxicological endpoints, which can further enhance disease diagnosis and screening. ● The developed model's read-across capabilities allow prediction of toxicity of similar nanomaterials based on their Euclidean distances, accelerating identification of potential disease risks associated with new or under-studied NMs. NC20 - Predictive toxicity assessment of semiconductor quantum dots that are used as fluorescence probes – adverse effects on the human lung epithelial carcinoma cell line A549 ("QD-cytotox") ● Nanomedicine and nano-based sensors are increasingly being utilised in health monitoring and control, and were critical to both the testing for, and vaccination against, Covid-19. ● Ensuring the safety of nanomedicines and nanosensors is critical: predictive models such as Quantitative Structure-Activity Relationship (QSAR) models to predict the health implications for nanomedicines are critical. Provision of user-friendly interfaces and detailed training materials,	- Many of the approaches developed in NanoCommons, especially around best practice in making research data and nanoinformatics software FAIR (Findable, Accessible, Interoperable and Reusable) have been further developed in other projects, including NanoSolveIT, CompSafeNano and MACRAMÉ, and are being systematised and documented as how-to guides via the WorldFAIR project, which aims to support global best practice within and between domains to support achievement of the SDG. SDG5: Gender equality - Despite progress in understanding of differences in disease susceptibility between sexes (e.g., women have double the risk for Alzhemier's disease than men) and differences in responses to drugs and medications, there are still major disparities in provision of tailored healthcare to women. The NanoCommons approaches, including biomarker discovery, biomolecule binding assays, determination of the Molecular Initiating Events leading to Adverse Outcomes and the associated Adverse Outcome Pathways (AOPs) can facilitate progress towards sex-considerations in design and testing of medicines, including nanomedicines, and through consideration of hormone and sex-specific interactions.

Applications of Nanotechnology	NanoCommons TA project: role of FAIR nanoEHS data and/or nanoinformatics in supporting the SDGs	How nanoinformatics data and/or tools directly or indirectly support the SDGs (not a 1:1 mapping but rather an overview for each of the goals)
	modelling-ready datasets, fully documented models and underpinning datasets, and best practice for these steps are key outcomes from NanoCommons relevant to multiple SDGs.	
Drug delivery systems	NC25 - Stochastic optimisation for grouping nanoPBPK model parameters and estimating their values: New methodology and service development ● nanoPBPK models are essential to predict the biodistribution of nanomedicines for example, to ensure they reach the target site and remain there for the required duration. ● Within NanoCommons the first compilation of nanoPBPK models was developed and these were made available for re-use and further development / parameterisation (to cover additional NMs for example) and bespoke models were also developed to fit users' needs. ● Providing user-friendly graphical interfaces and simplifying the processes for inputting parameters reduces training barriers and democratises access to models, predictions and progress. NC23 - PBPK model on 99m-Technetium labelled carbon nanoparticles inhaled by humans: Implementation in R and integration into NanoCommons modelling toolbox. ● The service provided here was re-coding of existing models into the mode accessible R programme, which also facilitated integration with other models into a modelling workflow. ● Providing user-friendly graphical interfaces reduced the need for coding skills and thus reduces barriers to access / democratizes access. ● Integration of the re-coded models into the NanoCommons	SDG1: No poverty - The PBPK, QSAR and other predictive models developed in NanoCommons can be re-parameterised for different organisms, and re-purposed for design of anti-viral agents, such as anti-fungals to reduce pest impacts on crop production and thus increase food security and small-farm profitability through reduced crop losses. - The democratisation of data and modelling tools for nanosafety assessment and Safe and Sustainable by design nanomaterials development, as pioneered by NanoCommons, is an important step towards levelling the playing field and thus reducing poverty through access to innovation, education and ability to tailor approaches to the local conditions. SDG9: Industry, innovation & infrastructure - Start-ups and community innovation clusters rarely have access to specialist knowledge and computational expertise. Democratising access to nanoEHS tools and datasets enables responsible choices whilst supporting local innovation potential. The breadth of application areas for data-driven modelling, and safe-by-design materials are endless, and sharing of knowledge and cross-fertilisation of normally disparate industry sectors offers enormous potential for innovation. Infrastructure projects, like NanoCommons offer a platform for connecting ideas and people, through provision of tools, networking, training opportunities and expertise to support implementation and operationalisation.

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	modelling toolbox ensures stability of access and sustainability.	
Air pollution and remediation	NC16 - Data capturing, storage and management of high quality, curated and harmonized data generated under the ASINA project while increasing fairness scores ● Field Exposure Monitoring (FEM) campaigns produce a significant amount of data that are valuable for emissions, exposure and risk assessment, as well as providing insights into the factors affecting process emissions, exposure levels and risks. ● Using the data shepherding approach, the TA provided an annotated template for capturing FEM data, and increased their interoperability, and re-usability for exposure and risk assessment (18). ● Applicability for assessment of occupational exposure during production to provide safer workspaces and protect health. NC10 - Structural alterations of allergen upon nanoparticle binding ● Allergens are increasingly prevalent in the environment, including pollen. ● Through combination of experimental and computational data, new insights into interactions of allergens with nanomaterials were gained, and increasingly predictive models were generated (16). ● Increased utility of the models for predicting protein (allergen) binding to nanomaterials and fully documented models to increase regulatory trust as models become increasingly validated.	SDG3: Good health and well-being - Collectively the projects that developed models for assessing / predicting impacts of nanoscale entities on living systems, whether intentionally destructive interactions (killing the virus) or unintentional impacts of materials designed for diagnostic or therapeutic effects, provide a strong starting point and best practice for development of additional models and understanding of health and well-being. Data and model sharing are critical to maximise translation of knowledge and to safe re-purposing of tools and approaches to new challenges, where existing approaches can be deployed rapidly to tackle new disease-related questions. SDG17: Partnerships for the Goals - NanoCommons's main objective was to build a community of practice, and the underpinning support to drive change in research culture, such that the management and sharing of data was moved to the point of data collection, rather than being something performed under duress at the end of the project, to fulfil funder mandates. The TA activities presented herein were a clear example of the benefits of partnership, whereby one party had a problem or research question to be addressed and the other had a potential solution that could be applied, tailored and tweaked to meet the research need. Scaling this up to addressing global challenges, demonstrates the need for actors who can connect needs and solutions, and an essential part of this is open and FAIR data and models, where re-use and derivation conditions are clear and foster growth and innovation.

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Construction	NC21 - Implementation and validation of the FAIR principle for data produced in SAbyNA project to ensure that high quality data is flowing into data repository ● As a case study within SAbyNA, 3D printing and paint are used, where exposure to nanomaterials is possible. Assessment of approaches to reduce exposure through application of SbD approaches. ● Via the TA, extensive knowledge building on FAIR data management workflows was provided. ● Data are being incorporated into the NanoCommons KnowledgeBase (data warehouse, (22)) to facilitate data re-use for modelling for occupational and consumer risk assessment. NC04 - Computational analysis of mesothelioma expression profiling data with Enalos Informatics Tool ● Occupational exposure is considered during construction, and especially during demolition of ulcer buildings where asbestos or other known toxic particles may be present. ● Open access modelling tool developed for analysis of mesothelioma expression profiling data to provide low-cost predictions of hazard. ● User-friendly graphical interfaces that reduce the need for programming skills are critical to democratise machine learning /AI.	SDG11 - Sustainable cities and communities - The mixture toxicity datasets and models, developed in NanoCommons or elsewhere, as represented by the *Daphnia magna* model, is an important step towards understanding the combined effects of pollutants in the environment, including the potential for nanomaterials to mitigate the impacts of other pollutants. Such data and models can be used as a basis for prioritisation of chemicals or for identification of pollution hot-spots for remediation, for example. - By understanding interactions between chemicals, and the combined effects of chemical mixtures on model organisms, approaches such as Safe-by-design can be applied as part of responsible innovation, to support safety and more sustainable chemicals and materials, while maintaining functionality. Making such data and tools available freely, as part of efforts to democratise access, supports industry and innovation.