

Deliverable report for

SUN Sustainable Nanotechnologies

Grant Agreement Number 604305

Deliverable D 1.2 SUN Project Database

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Lead beneficiary for this deliverable: Institute of Occupational Medicine - IOM

	Dissemination Level:	
PU	Public	
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
СО	Confidential, only for members of the consortium (including the Commission Services)	Х

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Description of task

Task 1.2 "Construct and maintain the SUN project database" Involved partners: IOM, UNIVE, all participants Responsible partner: IOM Duration: Month 12 - 42

1. Status of this report

Deliverable D1.2 is the final report on Task 1.2 "Construct and maintain the SUN database". It accumulates and finalises the account of the work carried out by the task from months 12 to 42. It will also describe the interactions that members of the SUN consortium had with other projects to coordinate and harmonise the efforts to enable data exchange, template, ontology and database development. Earlier interim reports have provided information on progress on an incremental basis. This version of the deliverable has been composed as a final deliverable at month 42 of the project, updating the previous month 36 version which was submitted in October 2016.

2. Overall aims and objectives of Task 1.2

All multi-disciplinary projects of significant size require a database to store and maintain the data generated by the project. The database development of Task 1.2 within WP1 was assigned to gather & collate all relevant data generated by WPs, with completeness, quality-checked, catalogued and stored suitably in the SUN project database, the project's data repository. The SUN database has been implemented as a searchable operational project database to store and maintain data generated by the project. All the relevant SUN data has been catalogued in a consistent fashion with the aim of relating methods (e.g. characterisation, dispersion etc.) with experimental results. The implemented database provides facilities to search, query and retrieve selected project datasets.

In principle, available raw data is part of the project and all partners can have access to other participants' data. Any usage of the SUN data while SUN progressed (e.g. for publications) was sanctioned by the SB and agreed by the author of the data. Access to SUN data by third parties, during the project lifetime, is subject to the usual confidentiality agreement with the SB and the relevant authors. At the end of the project, the SUN database will be made available to the EC.

Whilst the database "as is" is available with this report at delivery time, it is here noted that with some earlier delays to the actual timetable of data generation and return in the project, and following considerable prompting, we expect a few data files are still due for return, and for some data aspects that may be beyond the official Project end date; from previous experience that data may continue to be received after that time. So, in the interests of completeness we will still endeavour to add this to the SUN repository. It is anticipated that facilitating and developing further the channels for data sharing, following publication embargoes etc, will also

continue beyond the official life of the SUN project, in other further developments, again as it has for some other projects. We certainly aim to continue to facilitate this in the interests of SUN, subsequent projects where practicable and for the NANO-EHS community more widely. For the latter, in the course of doing the SUN work we have had ongoing liaison, sharing and other interaction with the eNanoMapper project and the Nano Safety Cluster (NSC) particularly through activities in WG4, Database Interest Group, and these also are described.

3. Description of work and achievements

The previous 36 month progress report for the SUN project database deliverable included detailed coverage of key work up to that point, including overall database design, template development, data gathering and liaison activities, and data returns to date. It reviewed several tasks and activities that have continued to take place since then. Thus, as a cumulative deliverable, all of the relevant parts of these activities are included here, supplemented with further results of the continuing work and the details of final output and achievements.

In the first period our work on the SUN project database was mainly concerned with developing two key areas. Firstly, the development of data collection templates and related resources for use by the scientists in the different major data generating parts of the project, as well as plans for their distribution and collection. Secondly we also prepared an initial schema and operating system for the operational database to be used to catalogue and manage the data received in the course of data collection as the project proceeded. It is here acknowledged that both of these tasks benefitted from our prior experience and resources developed earlier in the FP7 projects e.g. NANOMMUNE, NANEX, ENPRA and MARINA, where these resources were adapted and further developed for SUN. This has been extremely useful, as it allowed the expenditure of work on these early development tasks to be relatively modest, knowing that in SUN the number of data donors, the greater diversity of different dataset types being generated, and the total to be collected overall would require significant efforts to be devoted to the data collection, collation and data management tasks.

In broad summary, having earlier established the foundations of our approach for this deliverable and the means of achieving it, in the interim practical database implementation work and actual project data collection has been on-going whilst some partners have completed, and others have been continuing to carry out experimentation and data generation activities. We have continued liaison with the relevant partners, and early in 2015 built on the earlier template formats where appropriate feedback or experimental or test developments have required this. This was just prior to a data procurement exercise (in summer 2015) that saw a cycle of WP1 circulating and reminding participants to fill data templates, for return as soon as possible to WP1. Data procured has been added to the database, and when ready will be forwarded for use by others in the project.

It is acknowledged here that the development of aspects of these resources and techniques (e.g. templates, database design and collection methods) has benefitted from and built upon

the foundations laid by prior experience and resources developed in the earlier FP7 projects, NANOMMUNE, NANEX, ENPRA and MARINA, although the diversity and variability of requirements in the SUN project were considerably more than in those earlier projects.

The sections that follow have been updated with the results of incremental and cumulative activities since the previous report. In this last period there has, as anticipated, been a marked increase in the more time-consuming practical data collection activities with ongoing data processing, management and database loading being carried out. Whilst the database design and structures are completed, and the vast bulk of relevant data has been returned by partners and added to the database, at time of writing we are aware that there are still small amounts of data in some areas of the project that is still being finalised. We are hopeful of receiving some of this data from some partners as the project closes and wherever possible we will endeavour to add that information to the database.

4. Project template development for data recording and curation

In order to assess requirements, plan for the SUN database and make it available for use by others, we have liaised with WP Leaders in an incremental fashion as the project has evolved and progressed. This has allowed us to build a more complete and up-to-date inventory of the data being produced or collected during the project as the work packages have evolved and developed. To help build up such an inventory initially, and to provide data collection materials, IOM have developed various data collection forms and templates, which have been distributed to the relevant WPs.

In the early stages of the project, these practical efforts necessarily concentrated on the characterisation (WP1), ecotoxicology (WP4) and toxicology (WP6) work packages, liaising and interacting with them during the development of their practical work. Subsequent liaison sought engagement with other WPs on Exposure and Release data and their relatively less structured and more qualitative types of data and information. The information provided allowed us to generate an overall inventory for SUN data with respect to the types of data to be generated, their expected formats, approximate volumes and anticipated timelines for data gathering and return. We have used this (regularly updated) information to periodically remind and follow up with the participants in order to obtain their data.

In terms of formal data template developments the most significant expenditure of effort in this respect has been on data requirements for the toxicology and ecotox areas of the project. WP1 has worked closely with members of WP6 on the development and use of data collection templates and recording forms for in-vitro and in-vivo results. In these areas we have, as planned, further developed materials and resources derived from earlier IOM FP7 toxicology templates. These templates were used to collect project data in ENPRA and MARINA, and they have been adapted and extended for SUN purposes. Specifically, in an intensive period of work the templates were adapted and rearranged for new assay types, with higher volumes of samples, and much altered data lay-outs than those encountered previously (with P26, KI, also

an eNanoMapper partner). These discussions and adaptations also allowed for the integration of efficient dose-response analysis in WP6 via the PROAST model (with P25 and P26, for in-P16 for and of vitro. and in-vivo), training in the use PROAST. (www.rivm.nl/en/Documents_and_publications/Scientific/Models/PROAST). It is worth noting that mutual benefit was derived from project interactions between SUN and NanoSolutions in this area, as well as later on with eNanoMapper. In addition, modified versions of the toxicology templates were developed for ecotox data, through liaison and input from WP4. WP1 also adjusted and supplied physicochemical characterisation data collection templates to UNIVE and VN for their results early on in the project. In the event, whilst the templates helped in data definitions, in this instance T1.2 extracted the data from the deliverable documents for the database.

Following alterations to project plans and experimental designs in some WPs, and related delays in results being made available, after year one WP1 prepared and distributed more general data collection forms for circulation to the Consortium. These were sent with accompanying explanatory information and guidance by email to the WP leader, or to the WP's nominated "Data Coordinator", a selected area expert on the data being produced. This was agreed through discussion with WP Leaders and candidate coordinators at the 1st SUN Annual Meeting (22 – 23 October 2014, Utrecht). Since then through further ongoing discussions with as many relevant partners as possible and assisted and motivated by UNIVE as project coordinator in WP1, we have continued data collection efforts on an ongoing basis, with mixed results in different WPs. As usual as the project progressed changes in substances, experimental designs and timetables delayed some data productions. Following further encouragement at the October 2015 meeting a revised data collection survey was distributed, and subsequently followed up periodically. This received further encouragement after the October 2016 meeting, and was followed up by further reminders to return data and information to WP1.2.

Regarding physical file handling, to improve on prior experience by encouraging greater standardisation and make like easier for all concerned, we also advocated more systematic naming convention for the template and data files to encourage the consistent use and identification of the files and their contents. This embeds the Work Package ID, Partner ID, ENM, End point-assay type, and Cell type into the file name. Users were strongly recommended to follow this pattern, and this has proven to be largely, though not universally, successfully adopted.

Appendix 1 shows the significant data collection templates and formats used in the project for data recording, collection and curation.

5. Data collection from SUN partners

WP1.2 has continued liaison with the relevant WP partners on an ongoing basis, establishing the general description and overview of their work programme i.e. studies, experiments,

assays, test method descriptions, SOPs, model development, results output and other generated SUN data. Data procured has been added to the SUN database.

The actual work in the data gathering tasks has been concerned with the following:

- Distribution of initial information gathering templates to identify and gather general work programme overview, ongoing collaboration and building inventory of data received from all Work Packages
- Further work on data collection templates and use by the scientists in the different data domains of the project, as well as continuing liaison for their distribution and collection
- Screening/validating for completeness and overall quality of data templates received
- Implementation of the database structure, user interface design and related development for the operational database being used to catalogue and manage datasets received as the project has proceeded.

To enhance the return of data to the repository the appointment of recognised "data coordinators" for WPs, in order to help liaise and take responsibility over the details of different data types and the transmission of results data has been very helpful and effective. Going forward it is a practice that should be applied in WPs of all data-generating projects, specified in good data management planning (in a Data Management Plan (DMP), as is now a requirement in H2020).

The support of the WP1 Project Coordinator to strongly encourage the data returns was also very helpful in providing necessary impetus with regard to the need for the partners to provide data. Such efforts continue in SUN, as there is still outstanding data to be returned and processed for the repository.

Overall, the approach we have adopted means that the data is collected, documented as far as possible based upon what is provided by SUN partners, and when ready made available for use or transfer to other parties. In earlier projects (NANOMMUNE, ENPRA, MARINA) we were mandated to forward datasets to the JRC - NanoHub database at the end of the project, so this is quite analogous to plans to forward suitable SUN data to an instance of the eNanoMapper database, following any data embargo period and the establishment of any necessary data sharing agreements, or other (legal) formalities required.

6. SUN database developments

In developing the SUN project database, WP1 has built upon and further developed techniques from earlier projects including those in ENPRA and MARINA, and as it was happening contemporaneously, has also included sharing of template materials and experience from the NANOSOLUTIONS project, as well as with the developers in the eNanoMapper project over the last three years. In order to address the wider data needs of SUN we have extended the domains of the earlier databases to cope with the greater diversity of data types found in SUN.

The result of these efforts is the "SUN Data Repository", including the database, relevant datasets, and related data management materials. The operational repository has been very well suited for ongoing project data management as it provides a catalogue and inventory that enables the collection, processing, and retrieval of project data, including:

- Experimental results on release, exposure, physicochemical properties of (Eco) toxicity, In-Vitro, In-Vivo and Exposure studies etc.
- Standard Operating Procedures (SOPs) and testing protocols.
- Standard database management and administration procedures including security, resilience and quality control.

In SUN, well before the advent of eNanoMapper and our interactions with it, our database strategy and plan was based on the earlier design, materials and experience of earlier projects (NANOMMUNE, ENPRA and MARINA), largely as a consequence of their success, and also in order to help achieve the task within the resources available, which were modest compared to the earlier projects, given the greater diversity of data types anticipated in SUN. Therefore, in brief, a similarly practical but necessarily "traditional" approach was planned, and has been followed. This has used the previous techniques and templates, with further adaptations, additions, and so on where necessary to adapt things to SUN purposes. The SUN repository database is populated with an inventory of project data, with details of all the datasets received, with links to the actual dataset and related documentation (SOP, or test method description form, etc.).

While we have been applying this basic database model efficiently for the SUN work, based upon earlier experience, it was also known that a very high proportion of the work would be expended in the practicalities of data collection and handling: in liaison and discussion with partners; agreeing and modifying templates for data capture where appropriate; suitably obtaining data (and chasing, reminding, etc.); checking, documenting and cataloguing the datasets from the various parties; all with considerable interaction with partners and frequently several iterations needed in order to achieve satisfactory final return of data. In addition, as they arose, interactions with other Nano-EHS community developments and the eNanoMapper project also required time and resource to execute.

A great deal of flexibility in the day to day approach to the database work in WP1 has been needed, although we have generally adhered to the principles of the WP1 database plan in order to facilitate as much data collection as possible within the available resources and to avoid unaffordable scope creep. We have repeatedly presented this approach, with schematics of the database methodology, in presentations to the MC, at project meetings, and in periodic reports, together with explanations of the reasons for this approach. However we have also naturally spent time and continued to interact with the wider generic data developments mentioned above, and other specific interactions with eNanoMapper developments as they have evolved, see outlined below. These interactions have similarly been outlined in our presentations and reports as the project has proceeded.

Strategically in SUN we adopted a similar general practical approach as that used in previous FP7 project data management, and build upon the foundation provided by our earlier MARINA (and other project's) work. We adapted, modified and tested assay templates with partners and also with eNanoMapper, which it was hoped could be the ultimate destination for much of this template data. With templates for data collection, we developed a very practical Operational Database to catalogue and collate together the SUN datasets and provide a simple and easy to use interface for their management, selection and retrieval, whilst at the same time maintaining the template format for provision to eNanoMapper. A schematic of the database operation is shown below in Figure 1 highlighting the main components and areas managed by the database and the aim of transferring appropriate datasets and documentation to eNanoMapper for upload.

The operational database is implemented as a Microsoft Access application for building and giving access to the main catalogue and uploaded study data, with the scientific results in template formats linked to the database records. This allows the database to document and track the data overall, and allows the template datasets to be readily provided to an eNanoMapper implementation. Once all of the data has been received and the database finalised, we will also publish a web-based version of the operational database, which will be available through the web link Sun.iom-world.co.uk. Ultimately this should be subsumed in an updated eNanoMapper database: we are collaborating with the more recent Horizon 2020 NanoReg2 (http://www.nanoreg2.eu) and caLIBRAte (http://www.nanocalibrate.eu/home) projects, aiming to transfer data to an updated eNanoMapper database implementation (see further in Sections 9 and 10 below).

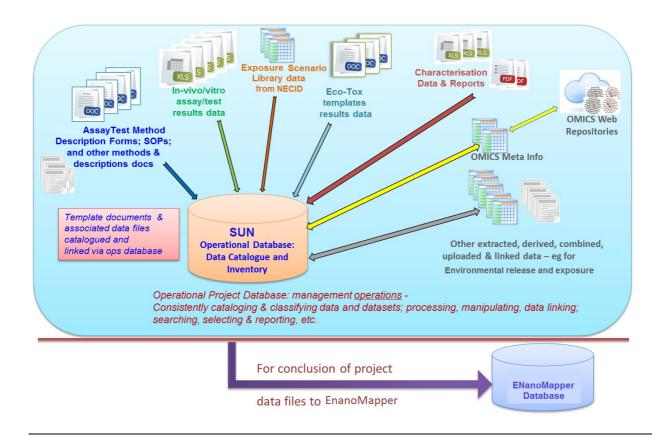


Figure 1: Schematic overview of content and operation of the database showing key data areas

In general the datasets have been incrementally added to the database as it has been received and screened. An interface to the catalogue and data was produced to allow a user to easily navigate the datasets and search and filter information for different areas. Figures 2, to 6 shows some example screen shots of the interface for the main menu, environmental release and exposure, ecotoxicology, occupational & consumer exposure and in-vitro toxicology data.

Sustainable Nanotechnolog	Operational Database						
Introduction to Operational Database & Repository data	Introductory information about the contents and use of the database						
WP1: Characterisation data	Phys-Chem characterisation data for SUN.						
WP2: Lifecycle thinking	Lifecycle Thinking						
WP3: Environmental release, fate and exposure	Environmental release, fate and exposure						
WP4: Ecotoxicology	Eco-Tox assay results, aggregated and summarised by Partner						
WP5: Occupational and consumer exposure	Occupational and consumer exposure						
WP6: Toxicology and human health risk (In-Vitro)	In-Vitro assay information & results returned by WP partners						
WP6: Toxicology and human health risk (In-Vivo)	In-Vivo assay information & results returned by WP partners						
WP7: Safe production, handling and disposal	Safe production, handling and disposal						
OMICS Data	OMICS results - linked to online project repositories						
Exit							

Figure 2: Opening menu of SUN Operational Database

SI	JN WP3 -	- Environn	nental release, fate and	exposure					
				umn field to filter by and se umn and select 'Remove filt		By Selection' or salso available of			
D	Partner	Task	Experiment Name	Key Aims and Objectives	Type of Output datasets	Approx Dates	Deliverable	Related data files	
1	BASF	Task 3.2	Weathering of Fe2O3_PE_USE and PE_USE (protocol adapted from ISO 4892- 2:2009-11)	Characterize the degradation of PE nanocomposite upon weathering.Quantify the release of Fe2O3 NOAA upon weathering.	Release rate (ie numerical data in mg.m- 2)FTIR spectra (27)XRD diagrams (7)Crystallite sizeX- ray computed microtomorraphy.(4)	Start : 08/14 End : 12/16	D3.1	Release rates : 2015 02 20 ICP-MS Fe Lixi A&D Fe203_PE_USE FreeFe xlsx 2015 06 15 ICP-MS Lixi Suntest A&D Fe203_PE_USE TotFe xsix FTIR analysis: 2016 12 06 Fe203_PE spectres corriges xlsx 2016 12 06 Fe203_PE spectres corriges xsix 2016 12 06 FE_USE spectres corriges xsix	
2	RWTH	Task 3.3	Weathering of Fe2O3_PE and PE fragmented products	Compare weathering of bulk materials and fragmented productsProduce weathered fragmented product for use in other work packages	WFP massFTIR spectra (8)XRD diagrams (8)Crystallite sizes (12)	Start: 02/15 End: 04/15	D3.1	2016 12 06 FTR FP weathering xsix 2015 07 SUN_DRX FP_8w_12w.ppt	
3	UNIVIE	Task 3.1	HNO3 dissolution and reductive dissolution of surface-available Fe in Fe2O3_PE_FOR and Fe2O3_PE_FP_USE	Define a reliable method to quantify surface-available Fe in lixiviates obtained from weathering experiments	Extraction yields (3)Surface available fraction (2)	Start: 01/15 End: 03/15	D3.2	2015 02 10 ICP-AES Fe Tests Extractions H2O + HN03.xstx 2015 02 11-12 ICP-AES Fe Mineralisations MW290115.xstx 2015 02 12 ICP-AES Fe Extractions CBD 01 15.xstx	
4	UNIVIE	Task 3.1	Mineralization of PE matrix	Validate method for quantification of total Fe released in the lixiviates of weathering experiments	Fe concentration in solids samples (3)	Start: 01/15 End: 02/15	D3.2	2015 02 11-12 ICP-AES Fe Mineralisations MW290115.xstx	
5	UNIVIE	Task 3.1	Separation of CuO NOAA adsorbed in sediments	Validate a method for reliable extraction of CuO NOAA from sediments	Size distributionsCu recovery rates (6)	Start: 02/15 End: 07/15	D3.2	CENT) CuO Spiked Sediment Data xsk	
6	BASF	Task 3.2	Weathering of wood blocks coated with CuO_AcryI_FOR and AcryI_FOR (protocol adapted from EN 927-	Characterize the degradation of CuO_paint upon weathering.Quantify the release of Cu upon weathering and determine	Release rate (ie numerical data in mg.m-2)	Start: 04/15 End: 12/16	Data not reported under D3.1 due to delays in	2015 09 ICP-MS Cu Ti - CuO_acryl Lixiviates.xstx	

Figure 3: Example records of Environmental release and exposure data

	Partner					·	also available on T		71107 51	
-			NM Substance	Lab name	Assay / End Point Name	CellType	CellTypeDesc	Assay File	TMDF File	_
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- ALAMAR_24w_longterm.xls	SUN-Ecotox-CLC-CuO- WP4_P15_Test_24w_longterm.do	
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- CFDA_24w_longterm.xis	SUN-Ecotox-CLC-CuO- WP4_P15_Test_24w_longterm.do	
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- NR_24w_longterm.xls	SUN-Ecotox-CLC-CuO- WP4_P15_Test_24w_longterm.do	
	INIA	P15	Cuso4 Salt	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- ALAMAR_24w_longterm.xls]	_
	INIA	P15	Cuso4 Salt	Department Of Environment	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- CFDA_24w_longterm.xls]	
	INIA	P15	Cuso4 Salt	Department Of Environment	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- NR_24w_longterm.xls]	
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- ALAMAR_96w_24h.xis	SUN-Ecotox-CLC-CuO- WP4_P15_Test.docx	
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- CFDA_96w_24h.xls	SUN-Ecotox-CLC-CuO- WP4_P15_Test.docx	
	INIA	P15	Cuo_1_np_syn	Department Of Environment	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP- NR_96w_24h.xis	SUN-Ecotox-CLC-CuO- WP4_P15_Test.docx	
ס	INIA	P15	Cuso4 (ion Control)	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- ALAMAR_96w_24h.xls]	
1	INIA	P15	Cuso4 (ion Control)	Department Of Environment	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- CFDA_96w_24h.xls]	
2	INIA	P15	Cuso4 (ion Control)	Department Of Environment	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuSO4- NR_96w_24h.xls]	
3	INIA	P15	Cuo_101_sol_bm_syn	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP_101- ALAMAR_96w_24h.xis	SUN-Ecotox-CLC-CuO_101- WP4_P15_Test.docx	
4	INIA	P15	Cuo_101_sol_bm_syn	Department Of Environment	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP_101- CFDA_96w_24h.xls	SUN-Ecotox-CLC-CuO_101- WP4_P15_Test.docx	
5	INIA	P15	Cuo_101_sol_bm_syn	Department Of Environment	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP_101- NR_96w_24h.xls	SUN-Ecotox-CLC-CuO_101- WP4_P15_Test.docx	Ī
'	INIA	P15	Cuo_102 _sol_bm_cit_syn	Department Of Environment	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP_102- ALAMAR_96w_24h.xls	SUN-Ecotox-CLC-CuO_102- WP4_P15_Test.docx	
ภ	INIA	P15	Cuo_102 _sol_bm_cit_syn	Department Of Environment	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio)	SUN-ECOTOX-CellTestAssay_CLC-CuONP_102- CFDA_96w_24h.xls	SUN-Ecotox-CLC-CuO_102- WP4 P15 Test.docx	Ĩ

Figure 4: Example records of ecotoxicology data

			onal and Consum												
			ords, right click on t r(s), right click on tl						or 'Sort asc/desc on Toolbar abov			View all the Measurements	View a Append		2
D	ENM	Workers No	Activity	Location	Source Domain	Automation Level	Exp Situation	Exp Pattern	Activity Duration	Sample Type	Aactivity Desc	Segregation	General Ventilation	Distance	Product Name
1	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal		00:22:00	Personal	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	Catalyst
2	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal		00:22:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	Catalyst
3	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal		00:22:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	Catalyst
4	MWCNT	10 - 19 Workers	Transfer of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:07:00	Personal	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	Catalyst
5	MWCNT	10 - 19 Workers	Transfer of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:07:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	Catalyst
6	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:03:00	Personal	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	metal- hydroxides
7	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:03:00	Personal	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	metal- hydroxides
8	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:03:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	metal- hydroxides
9	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:03:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	metal- hydroxides
10	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Manual without restrictions	Normal	Occasional	00:03:00	Static	Handling of the catalyst	None segregation	Mechanical ventilation -	0,5 m	metal- hydroxides
11	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Personal	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes
12	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Personal	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes
13	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Personal	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes
14	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Personal	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes
15	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Personal	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes
16	MWCNT	10 - 19 Workers	Falling of powders or granules	Area indoor	Handling and transfer of bulk	Semi automatic	None		00:01:00	Static	Handling of the catalyst	None segregation	None ventilationN	0,5 m	Carbon nanotubes

Figure 5: Example records of occupational & consumer exposure data

		rrent filter(s), right click on				(commands also availa			_
	WP Partner	NM Substance	Assay/End Point	Type ay Desc	Cell Type	Cell Line Desc	Assay Results File	Assay Test Method Description File	
10	WP P2 SIs 6 5 Wp		Fluorescence Measurement Of	Alamar Blue	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	SUN_WP6_AlamarBlue_CuO_C3A.xlsx	NanSol-TMDF-WP6-HWU25- CellViability-AlamarBlue-C3A.doc	
11	WP P2 Sls 6 5 Wp		Fluorescence Measurement Of	Alamar Blue	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	SUN_WP6_AlamarBlue_WCCo_C3A.xls	NanSol-TMDF-WP6-HWU25- CellViability-AlamarBlue-C3A.doc	
18	WP P2 Sls 6 5 Wp		Fluorescence Measurement Of	"fpg" Modified Alkaline Single	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	CoCl2.xlsx		
19	WP P2 Sls 6 5 Wp		Fluorescence Measurement Of	"fpg" Modified Alkaline Single	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	CuO.xlsx		
20	WP P2 Sis 6 5 Wp		Fluorescence Measurement Of	"fpg" Modified Alkaline Single	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	CuSo4.xlsx		
22	WP P2 Sis 6 5 Wp		Fluorescence Measurement Of	"fpg" Modified Alkaline Single	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	interference.xlsx		
23	WP P2 Sis 6 5 Wp		Fluorescence Measurement Of	"fpg" Modified Alkaline Single	C3a	Hepg2/c3a (atcc® Crl- 10741™), Derivative Of	WCCo.xisx		
25	WP P2 Kar 6 6 ska	blin Copper Oxide Nanoparticles	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_CuO_Raw264.7_AlamarBlue_C ytokine.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
4	WP P2 Kar 6 6 ska	olin Fp7-sun Priority Pristine Nanomaterials	Luminex		RAW 264.7	Mouse peritoneal macrophages	FP7SUN_Luminex_RAW264.7_2016.xls	SUN-TMDF-WP6- CytokineMultiplex_KI.doc	
6	WP P2 Kar 6 6 ska	olin Multi-walled Carbon Nanotubes	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_MWCNT_Raw264.7_AlamarBlu e_24h.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
7	WP P2 Kar 6 6 ska	olin Multi-walled Carbon Nanotubes	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_MWCNT_Raw264.7_AlamarBlu e_48h.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
8	WP P2 Kar 6 6 ska	olin Fe2o3 P Red 101	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_Pred101_Raw264.7_AlamarBlu e.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
9	WP P2 Kar 6 6 ska	olin Orgp Red 254	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_Pred254_Raw264.7_AlamarBlu e.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
10	WP P2 Kar 6 6 ska	olin Silicon Dioxide	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_SiO2_Raw264.7_AlamarBlue.xl s	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
1	WP P2 Kar 6 6 ska	olin Tio2(in Acid Water)	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_TiO2 HCI_Raw264.7_AlamarBlue.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	
2	WPP2 Kar 66 ska	olin Tio2(in Monopropylene Glycol)	Cytotoxicity	Alamar Blue	Raw264.7	Mouse Macrophages	SUN_WP6_TiO2resin_Raw264.7_AlamarBl ue.xls	SUN-TMDF-WP6-P26-CellViability- AlamarBlue-RAW264.7.doc	Ĩ

Figure	6:	Example	records	of	In-vitro	assays.
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SUN Deliverable 1.2

7. Overview of data returns to WP1

After considerable interaction with the various work packages to obtain their data, particularly over the last 6 to 9 months of the project, a large number of datasets have been collected and added to the SUN database. This section summarises the data obtained by WP.

WP1: Case study value chains

SUN Characterisation PDF report of pristine nanomaterials for (Eco)toxicological testing (D1.4) data has been exported to Excel spreadsheets (Fig 7) and incorporated into the SUN operational database. An overall summary of primary characterization results is given in Table 1.

Introductory worksheet - Please t	treat this as read-only & do not alter the data in this spreadsheet file, which during the project is only for
limited distribution to SUN partner	rs, or approved others subject to confidentiality discussions and approval from project leader Danail Hristozov (danail.hristozov@unive.i
Do not alter or update the data in t	this edition; if you discover any errors, or anomalies, or have data to be added, please inform peter.ritchie@iom-world.org & shahzad.ra:
	SUN project as work progresses, in which case an update will be issued when necessary.
This flexible spreadsheet format of	can be used, allowing different data items and formats to be viewed and used by partners in the course of work.
The key sheets and their contents	s to date are:
WorkSheets: (Use the link to mo	ve directly to the particular sheet)
Samples List	Table 1. Details of each SUN sample, specifying material, SUN code, CAS-number and supplier.
Primar Char Summary	Table 2. Summary of primary characterization performed by each partner.
Primary Char Results Summary	Table 3. Summary of primary characterization results
TEM Primary Size Distribution	Table 4. Observation and measurement results of TEM primary size distribution.
TEM Micrographs	Table 5. Representative TEM micrographs and measured particle size distributions for selected samples.
Crystallite Size Phases	Table 3. Summary of primary characterization results
Dispersability Water Biological	Table 6. Water and biological medium dispersibility results. The results in italic are calculatet by do not taking in account the peaks from the
Z Potential	Table 7: Z-potential results in UP water and Table 8: Z-potential results at pH7.
Photocatalytic Activity	Table 9. Photocatalytic activity data indicated as photon efficiency.
Surface Area Pore Size	Table 10. Surface area and pore size results. Pore size analysis method are reported in brackets (BJH: Barrett, Joyner, and Halenda; AVG: Ave
Average Agglomeration No	Table 11. AAN for water dispersions and Table 12. AAN for biological medium dispersions
Surface Chemistry	Table 3. Summary of primary characterization results

 Table 1: Summary of primary characterization results

		ech- Iique	Fe2O3_1_ NP_PROD	CuO_1_ NP_PROD	MWCNT_1_ NP_PROD	SiO2_1_ NP_PROD	TiO₂ acid water_1_ NP_PROD	TiO ₂ monopropyle ne glycol_1_ NP_PROD	WC+Co_1_ NP_PROD	OrgPig_1_ NP_PROD
Primary six distribution Min- Ma (average) Mode (1st quarti 3rd quartil [nm]	ax Ie	ΈM	11-112 (37) 32 (2843)	3-35 (12) 10 (9.214)	Ø: 4-16 (8) 7.4 (6.79.2) L: 575-3462 (1543) 1020 (9201800)	3-27 (11) 9.5 (814)	1-15 (4) 3.2 (2.94.4)	1-5 (3) 2.8 (2.53.5)	23-1446 (170) 48 (69280)	14-151 (43) 26.3 (29.849.8)
Shape	Т	ΈM	Irregular rounded particles	Semi- spherical particles	Bent and partially entangled multiwalled	Irregular polyhedrons and some spherical particles	Very small irregular polyhedrons and some spherical particles	Very small irregular polyhedrons	Irregular polyhedral particles and some semi- spherical with edges	Irregular polyhedrons and some small semi- spherical particles
Average crystalli size [nm]	te X	(RD	40	9.3	Not measurable	(JRC-IHCP) Synthetic amorphous silicon dioxide, impurities of Bohemite	18 (43%) 6.8 (57%)	10.6 (14%) 3.2 (86%)	15.4	No database available
Crystallite phase (%)	es X	RD	Hematite 100%	Tenorite 100%	(Nanogenotox) carbon nanotubes	(JRC-IHCP) 22 nm	Main phases: Brookite and rutile; Third phase: a salt or an oxide	Mix of anatase, rutile and brookite	Tungsten carbide 100%	No database available

Dispersability in	DLS	177.3 ±	139.5 ±	(JRC-IHCP)	(ENPRA)	85.9 ± 1.3;	82.1 ± 4.8;	182.8 ± 21.5;	137.3 ± 4.6;
water: D ₅₀ [nm];		6.6;	4.6;	175.9 ± 4.5;	216;	19411	25117	31	41
average		39	346	2419	6036				
agglomeration									
number (AAN)									
Dispersability in	DLS	148.2 ±2.2;	85.2±2.7;	Not available	Not available	60.0 ± 2.6;	Unstable	315 ± 18;	84.4 ± 4.5;
modified MEM		23	77			6592	sample	159	9
provided by the									
Heriot-Watt									
University: D ₅₀									
[nm]; average									
agglomeration									
number (AAN)									
Z-potential in UP	ELS	+32.0 ± 0.7	+28.1 ±	Unstable	-37.6 ± 0.8	+39.3 ± 1.1	+32.9 ± 2.2	+7.1 ± 0.5	-20.8 ± 1.3
water [mV]			0.6	sample					
Isoelectric point	ELS	9.7	10.3	Unstable	1.8	In progress	In progress	<2	2.1
[pH]				sample					
Photocatalysis:	Methyl	Not	1.5x10 ⁻⁴	9.5x10 ⁻⁵	1.3x10 ⁻⁴	2.4x10 ⁻³	2.4x10 ⁻³	6.7x10 ⁻⁴	Not
photon efficiency	ene	measurable							measurable
[unitless]	blue	(pigment)							(pigment)
	degrad								
	ation								
Specific Surface	BET	22.6 ± 0.1	47.0 ± 1.7	From other EU	From other EU	Sample	Sample	6.6 ± 0.4	94 (from
Area [m² g ⁻¹]		30 (from		project	project	degradation	degradation		producer)
		producer)		339.3 ± 17.3	190.5 ± 4.0	during	during		
						degassing	degassing		
Pore sizes [nm]	BET	65 (from	13.5 ± 1.6	Not available	Not available	Sample	Sample	Non porous	80, 200 to
		producer	(BJH)			degradation	degradation		2x10 ⁵ (from
			23.0 ± 0.9 (AVG)			during	during		producer
						degassing	degassing		

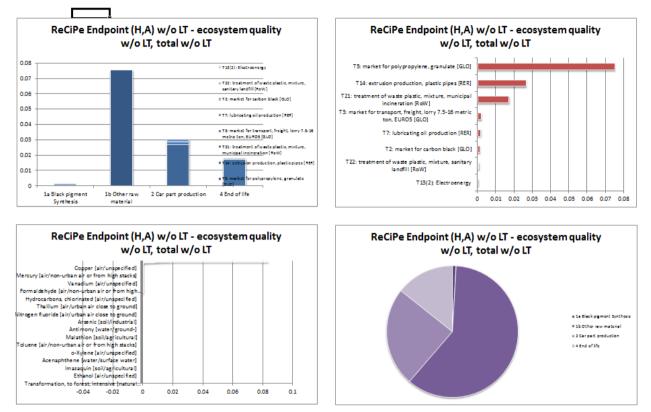
Surface chemistry	XPS	С	50.7	Cu =	Not available	(JRC-IHCP)	In progress	In progress	Co=0.08±0.01	C 77.1
[atomic fraction]		0	33.7	0.46±0.05		0 (72.1 at%), Si	_	-	W=0.05±0.01	0 10.9
		Fe	15.6	0 =		(25.0 at%) and			0=0.31±0.03	N 5.9
		(from		0.47±0.05		C (2.9 at%)			C=0.56±0.05	CI 6.1
		produ	cer)	C=		due to surface				(from
				0.07±0.01		contamination.				producer)
Structure	FT-IR	Match	with	Match with	(ENPRA)	Not available-	In progress	In progress	Match with O-	Match with
	and/or	Fe ₂ O ₃		CuO	High D/G				W-O bonds	Organic
	RAMAN	databa	ase	database	bands ratio:					Pigment Red
					high					254
					concentration					database
					of defects					
Chemical	ICP-MS	Cr:	32±2	Na:	Nanogenotox-1:	No element	Si:	Ag: 3.6±0.02	Co:	No efficient
impurities [mg kg [.]		Mass	loss	505±30	AI:	over 10	1143±137	Al: 2.8±0.6	83269±2213	sample
1]		in	TGA:	Pb: 36±2	42192±3352		Al: 4±1	As: 2.1±0.14	Fe: 1654±38	digestion
		-0.7%	from	Ag: 13±4	Co: 1911±274		Zn: 0.7±0.1	Zn: 1.3±0.08	Cr: 79±2	Mass loss in
		35°C	to		Fe: 3455±410;			Cu: 0.47±0.15	Cu: 14±2	TGA:
		800°0	2		Nanogenotox-2:			Co:	Mo: 12.7±0.2	-2.9% from
					AI:			0.36±0.001	Mn: 10.6±0.5	35°C to
					32627±13318			Cr:	Re: 6.6±0.2	315°C
					Co:1362±523			0.002±0.001	Ta: 5.3±0.1	
					Fe: 2667±973					

WP2: Lifecycle thinking

Life cycle assessment (LCA) of selected Nano products and associated materials (D2.3) and Umberto NXT LCA - Impact Assessment Analysis LCIA raw data including charts & pivot tables (fig 9) have been attached and uploaded to the SUN operational database (fig 8).

SUN WP2 - Lifecycle Thin	king	
D 2.3 - LCA of selecte	ed nanoproducts and associated materials	
Report and results compile	ed by WP2 (UniHB : P34)	
	mplements the life cycle perspective in the SUN case studies. In order to assess potential environmenta mpacts regarding each life cycle stage, the life cycle assessment (LCA) methodology is applied and the re compared.	
Deliverable Report		
Report Description	LCA of selected nanoproducts and associated materials	
Selected Case Studies:	Life cycle assessment (LCA) of selected Nano products and associated materials (D2.3) •Case study 1: Nano-WC-Cobalt (Tungsten Carbide-cobalt) sintered ceramics •Case study 2: Nano copper wood preservatives •Case study 3 and 4: CNT (Carbon Nano Tube) in plastics and CNT in anti-fouling bio-adhesion coating •Case study 5: SiO2 (Silicon Dioxide) as food additive •Case study 6: TiO2 (Titanium Dioxide) self-cleaning coating •Case study 7a and 7b: Organic pigment in plastics and Fe2O3 (Iron Oxide) pigment in plastics	
Report File Name	22062016_SUN_D_2_3.pdf	Open File
Output File	Umberto NXT LCA - Impact Assessment Analysis Raw LCIA data export with pivot tables	
Report File Type	Car_part_with_1_perc_CB_differenziert_ReCiPe_endpoints.xlsx	Open File
		Close Form

Figure 8: Life cycle assessment raw data and report



Umberto NXT Universal - Impact Assessment Analysis

Figure 9: Umberto NXT LCA - Impact Assessment Analysis charts

WP3: Environmental release, fate and exposure

Table 2 summarises the data returns from WP3 partners, which have been catalogued and linked to the database, giving a current total of 28 datasets.

Test Assay	Objective	Task	Output Description	Approx. Date	Related Excel Files	SUN Deliverable
Weathering of Fe2O3_PE_USE and PE_USE (protocol adapted from ISO 4892-2:2009-11)	Characterize the degradation of PE nanocomposite upon weathering.Quantify the release of Fe2O3 NOAA upon weathering.	Task 3.2	Release rate (ie numerical data in mg.m-2)FTIR spectra (27)XRD diagrams (7)Crystallite sizeX- ray computed microtomography (4)	Start : 08/14 End : 12/16	Release rates : 2015 02 26 ICP-MS Fe Lixi A&D Fe203_PE_USE FreeFe.xlsx 2015 06 15 ICP-MS Lixi Suntest A&D Fe203_PE_USE TotFe.xslx FTIR analysis: 2016 12 06 Fe203_PE spectres corriges.xlsx 2016 12 06 PE_USE spectres corriges.xslx 2016 10 10 OrgPig_PE spectres corriges.xslx 2016 12 07 Peak Area analysis_Fe203_PE.xslx FIT_IR.xslx XD: 2015 03 05 Bilan DRX.ppt X-ray computed microtomogaphy : Fig_tomo_vf.jpg	D3.1
Weathering of Fe2O3_PE and PE fragmented products	Compare weathering of bulk materials and fragmented productsProduce weathered fragmented product for use in other work packages		WFP massFTIR spectra (8)XRD diagrams (8)Crystallite sizes (12)	Start: 02/15 End: 04/15	2016 12 06 FTIR FP weathering.xslx 2015 07 SUN_DRX FP_8w_12w.ppt	D3.1
HNO3 dissolution and reductive dissolution of	Define a reliable method to quantify surface-available Fe in	Task 3.1	Extractionyields(3)Surfaceavailablefraction (2)	Start: 01/15 End: 03/15	2015 02 10 ICP-AES Fe Tests Extractions H20 + HN03.xslx 2015 02 11-12 ICP-AES Fe Mineralisations	D3.2

surface-available Fe	lixiviates obtained from				MW290115.xslx 2015 02 12 ICP-	
in Fe203_PE_FOR	weathering				AES Fe Extractions CBD 01 15.xslx	
and – –	experiments					
Fe2O3_PE_FP_USE						
Mineralization of PE	Validate method for	Task	Fe concentration in	Start:	2015 02 11-12 ICP-AES Fe	D3.2
matrix	quantification of total	3.1	solids samples (3)	01/15 End:	Mineralisations MW290115.xslx	
	Fe released in the			02/15		
	lixiviates of weathering					
	experiments					
Separation of CuO	Validate a method for	Task	Size distributions Cu	Start:	(CEINT) CuO Spiked Sediment	D3.2
NOAA adsorbed in	reliable extraction of	3.1	recovery rates (6)	02/15 End:	Data.xslx	
sediments	CuO NOAA from			07/15		
	sediments					
Weathering of wood	Characterize the	Task	Release rate (ie	Start:	2015 09 ICP-MS Cu Ti - CuO_acryl	Data not
blocks coated with	degradation of	3.2	numerical data in	04/15 End:	Lixiviates.xslx	reported
CuO_Acryl_FOR and	CuO_paint upon		mg.m-2)	12/16		under D3.1
Acryl_FOR (protocol	weathering.Quantify					due to
adapted from EN	the release of Cu upon					delays in
927-6:2007)	weathering and					paint
	determine under what					production
	form it is released.					
Weathering of wood	Quantify the release of	Task	Release rate (ie	Start:06/15	2015 11 ICP-MS Cu Ti - Lixiviates	Data not
blocks impregnated	Cu and compare it with	3.2	numerical data in	End: 12/16	CuAm-CuCO3.xslx	reported
with CuAmine and	Cu releases from CuO		mg.m-2)			under D3.1
CuCO3 (protocol	enriched paint.					due to
adapted from EN						delays in
927-6:2007)						CuCO3
						supplies
Aging of CuO NOAA	•	Task	• • • • •	Start:	Aging of CuO NP Data Tables_LS.xslx	D3.4
in Volvic water	possible	3.5	potential vs time	06/15 End:		
	transformation of CuO		(7)Cu dissolution	07/15		

		NOAA in mesocosms experiments		rate (3)			
CuO_AcryI_FOR a AcryI_FOR milling	nd	Develop a method to produce suspensions fragmented products from acrylic and CuO paintsCharacterize the obtained FP suspensions	Task 3.3	Size distributions	Start: 06/15 End: 10/15	2015 07 Paint milling synthesis.xslx	D3.4 MS6
•	ith nd	Determine environmental fate of CuO NOAA and CuO_paint FPs (=released NOAA)	Task 3.5	Cu concentration in different compartments (water, sediments, organisms)Cu distribution inside mesocosms systemsCu dissolution rateCuO NOAA biotransformation	Start: 10/15 End: 12/16	Cu concentrations and distribution: 2016 07 05 ICP-MS CE CuO.xslx 2016 09 12 ICP-MS Sed_CuO.xslx 2016 11 28 ICP-MS Mesocosmes CuO-Org.xslx Physico-chemical monitoring : Phys-chem parameters mesoCuO.tif	D3.4
CS with CN Concentrations CS Case Study	IT, =	Concentrations	Task 3.7	5 R files (*.Rda) Probability distributions simulations arranged in a matrix of 8 rows and 100,000 columns.	Start Date March 2016 September 2016	(*.RDA)	D3.7
CS with Copp Oxide, Concentrations)er	Concentrations	Task 3.7	4 R files (*.Rda) Probability distributions simulations	Start Date March 2016 September	(*.RDA)	D3.7

			arranged in a matrix of 8 rows and 100,000 columns.	2016	
CS with DPP, Concentrations	Concentrations	Task 3.7	5 R files (*.Rda) Probability distributions simulations arranged in a matrix of 8 rows and 100,000 columns.	Start Date (*.RDA) March 2016 September 2016	D3.7
CS with Iron Oxide, Concentrations	Concentrations	Task 3.7	5 R files (*.Rda) Probability distributions simulations arranged in a matrix of 8 rows and 100,000 columns.	Start Date (*.RDA) March 2016 September 2016	D3.7
CS with Silica Dioxide Concentrations	Concentrations	Task 3.7	5 R files (*.Rda) Probability distributions simulations arranged in a matrix of 8 rows and 100,000 columns.	Start Date (*.RDA) March 2016 September 2016	D3.7
Summary file	Summary information of the data delivered.	Task 3.7	1ExcelfileSummarystatistics(meanvalues)ofthedistributionsgeneratedanddescription	Start Date Task_3_7_data_summary.xlsx March 2016 September 2016	D3.7

			on how to access to		
			the R		
			files.		
Production of 14C-	Embedding of 14C-	Task		PP: 04/14-	D3.1
	0		•	,	D3.1
MWCNT/PP and		3.2	dispersion state of MWCNTs in PP and	-	
ероху	epoxy in order to			Epoxy:	
nanocomposites	produce composites		Ероху	07/15-	
	comparable to the			10/15	
	product used in the				
	case studies				
Release of 14C-	Measuring of release of			PP: 02/15-	D3.1
MWCNT/PP and		3.2	release data (in % of	06/15	
epoxy fragments	composites (0, 30 and		embedded 14C-	Ероху:	
from radiated	90 d of radiation) after		MWCNTs)	10/15-	
nanocomposites	different levels of			01/16	
after mechanical	mechanical treatment				
treatment	(knocking, shaking in				
	water, wiping)				
Release of 14C-	Measuring of release of	Task	EXCEL Sheet with	PP: 07/15-	
MWCNT/PP and	radioactivity from	3.2	release data (in % of	02/16	
epoxy fragments	untreated & radiated		embedded 14C-	Ероху:	
from radiated	composites in fresh		MWCNTs)	02/16-	
nanocomposites in	and sea water at			08/16	
fresh and sea water	several time points				
	(max. 210 d, 60 rpm)				
Release of 14C-	Measuring of release of	Task	EXCEL Sheet with	PP: 11/15-	
MWCNT/PP and	-	3.2	release data (in % of	04/16	
epoxy fragments	untreated & radiated		embedded 14C-	Ероху:	
from radiated	composites in quartz		MWCNTs)	02/16-	
nanocomposites in	sand at several time			06/16	
sediment (quartz	points (max. 100 d, 60				
()	, , , , , , , , , , , , , , , , , , , ,				

sand)	rpm)			
Release of 14C- MWCNT/PP and epoxy fragments from radiated nanocomposites in soil (Refesol 02 A)	Measuring of release of radioactivity from untreated & radiated composites in soil at 63 and 188 d, Mineralization of radioactivity Analysis of the shape of the released	Task 3.2 Task 3.2	release data (in % of embedded 14C- MWCNTs)	
epoxy composites and fragments via SEM and TEM after each release experiment	material (containing MWCNTs or free MWCNTs) and the	5.2	and surfaces of the nanocomposites by means of SEM/TEM	Epoxy: 01/16- 06/16
Production of MWCNT/PP and epoxy WFP from FP	Weathering of FP by radiating fragmented products with simulated sunlight (90 d, 50 W/m ²) to weathered fragmented product (WFP)	Task 3.3		PP: 04/15- 08/15 Epoxy: 01/16- 04/16
Release of Fe2O3 NOAA serving as pigments in polyethylene	Measure dissolved and nanoparticulate iron released in water media and calculate leaching rates	Task 3.5	Type of datasets: tables reporting mass concentrations of dissolved iron and number concentrations of	01/15 – 170203_SUN_AgNP-dissolution.xlsx D3.4 11/15 Data_Inventory_UNIVIE.xlsx method_schematic.pdf

			particulate iron; deliverable reports. Number of datasets: 2			
Release of CuO NOAA incorporated in antifungal paints (wood preservative coating)	Measure dissolved and nanoparticulate copper released in water media and calculate leaching rates	Task 3.5	Type ofdatasets:tablesreportingmass concentrationsofdissolvedcopperandnumberconcentrationsofparticulatecopper;deliverablereports.Number ofdatasets:2	01/15 - 11/15	- 170203_SUN_AgNP-dissolution.xlsx Data_Inventory_UNIVIE.xlsx method_schematic.pdf	D3.4
Release of surface- available CNT NOAA incorporated in epoxy matrix	Determine the amount of CNTs on the surface of the epoxy material	Task 3.5	Typeofdatasets:tablesreportingmassconcentrationsofdissolvedironandcobalt;deliverablereports.NumberNumberof2	01/16 - 04/16	- 170203_SUN_AgNP-dissolution.xlsx Data_Inventory_UNIVIE.xlsx method_schematic.pdf	D3.4
Release of surface- available CNT NOAA incorporated in polypropylene matrix	Determine the amount of CNTs on the surface of the PP material	Task 3.5	Typeofdatasets:tablesreportingmassconcentrationsofdissolvedironandcobalt;deliverablereports.NumberNumberof2	01/16 - 04/16	- 170203_SUN_AgNP-dissolution.xlsx Data_Inventory_UNIVIE.xlsx method_schematic.pdf	D3.4
Release of surface	Determine the amount	Task	Type of datasets:	01/16 -	- 170203_SUN_AgNP-dissolution.xlsx	D3.4

available Fe203	of Fe2O3 nanoparticles	3.5	tables	reporting	04/16	Data_Inventory_UNIVIE.xlsx
NOAA serving as	on the surface of the		mass cond	centrations		method_schematic.pdf
pigments in	PE material		of dissol	ved iron;		
polyethylene			deliverable reports.			
			Number of	f datasets:		
			2			

WP4: Ecotoxicology

The ecotoxicology summary results files, with a variety of test types received, have been catalogued and linked to the database giving a current total of 187 tests and assay results datasets as shown in Table 3.

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Cnt	Springtails Tests	F Candida	Folsomia Candida	1
Cocl2 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cocl2 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cocl2 Salt (ion Control)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cocl2 Salt (ion Control)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cocl2 Salt (ion Control)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cocl2 Salt (ion Control)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Copper Oxide Nanoparticles	Zebrafish Embryo Test	Zebrafish Embryos	Danio Rerio	3
Copper Sulphate	Zebrafish Embryo Test	Zebrafish Embryos	Danio Rerio	3
Cuo	Potential Ammonium Oxidation (iso 15685:2012)			8
Cuo	Springtails Tests	F Candida	Folsomia Candida	1
Cuo_1_np_pei Cuo_1_np_pvp; Cuo_1_np_citrate;	Multispecies Test		F. Candida, P. Minuta, H. Assimilis And M. Macrochaeta, H. Aculeifer, E. Crypticus	1

Table 3: Summary of WP 4 Ecotoxicology Test results returned and added to database

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Cuo_1_np_ascorbate				
Cuo_1_np_syn	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_1_np_syn	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	2
Cuo_1_np_syn	Earthworm In Vitro Tests	Coelomocytes	Eisena Fetida	1
Cuo_1_np_syn	Earthworm Tests	E Fetida	Eisena Fetida	2
Cuo_1_np_syn	Lymanea Stagnalis Acute Lethal Tests	L. Stagnalis	Lymnaea Stagnalis	1
Cuo_1_np_syn	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	2
Cuo_1_np_syn	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	2
Cuo_1_np_syn	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	3
Cuo_1_np_syn	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	2
Cuo_1_np_syn	Multispecies Test		F. Candida, P. Minuta, H. Assimilis And M. Macrochaeta, H. Aculeifer, E. Crypticus	1
Cuo_101_sol_bm_syn	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_101_sol_bm_syn	Cell Membrane Integrity (cfda-am)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_101_sol_bm_syn	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_101_sol_bm_syn	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_101_sol_bm_syn	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_101_sol_bm_syn	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_102 _sol_bm_cit_syn	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_102 _sol_bm_cit_syn	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_102 _sol_bm_cit_syn	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_102 _sol_bm_cit_syn (mo With Citrate)	dified Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_102 _sol_bm_cit_syn (mo With Citrate)	dified Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_102 _sol_bm_cit_syn (mo With Citrate)	dified Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_104_sol_bm_pei_syn (modified With Pei)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Cuo_104_sol_bm_pei_syn (modified With Pei)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_104_sol_bm_pei_syn (modified With Pei)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_104_sol_bm_pei_syn (modified With Pei)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_104_sol_bm_pei_syn (modified With Pei)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_104_sol_bm_pei_syn (modified With Pei)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuo_105_sol_bm_asc_syn (modified With Ascorbate)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuonm	Enchytraeus Crypticus	E Crypticus	Enchytraeus Crypticus	3
Cuonm	Enzyme Actitivy Patterns (iso/ts 22939:2010)			11
Cuonm	Microresptm			13
Cuonm	Potential Ammonium Oxidation (iso 15685:2012)			3
Cuo-nm	Potential Ammonium Oxidation (iso 15685:2012)			1
Cuo-np	Oecd Guideline 209			1

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Cuso4	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuso4	Lymanea Stagnalis Acute Lethal Tests	L. Stagnalis	Lymnaea Stagnalis	1
Cuso4	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuso4	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuso4 (ion Control)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 (ion Control)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 (ion Control)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 Salt	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 Salt	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 Salt	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Cuso4 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuso4 Salt (ion Control)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Cuso4 Salt (ion Control)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fe2o3	Oecd Guideline 209			1
Fe2o3_1_np_syn (pig Red101)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fe2o3_1_np_syn (pig Red101)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fe2o3_1_np_syn (pig Red101)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fe2o3p.red101	Potential Ammonium Oxidation (iso 15685:2012)			1
Fecl3 (ion Control)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Fecl3 (ion Control)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Fecl3 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fecl3 Salt (ion Control)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Fecl3 Salt (ion Control)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Fecl3 Salt (ion Control)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Feo2	Potential Ammonium Oxidation (iso 15685:2012)			1
Irgazin_pristine (org P.red 254)	Enchytraeus Crypticus	E Crypticus	Enchytraeus Crypticus	1

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Irgazin_used (org Pig_1_pp_use_fp)	Enchytraeus Crypticus	E Crypticus	Enchytraeus Crypticus	1
Iron Oxide Pigment	Springtails Tests	F Candida	Folsomia Candida	1
Lp 17206	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp 17206	Lysosomal Activity (neutral Red)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp 17206	Metabolic Activity (alamarblue)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp 17623	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp 17623	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp 17623	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Lp 17623	Metabolic Activity (alamarblue)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Lp17206	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Lp17206	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Lp17206	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Lp17623	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Lp17623	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Mwcnt	Potential Ammonium Oxidation (iso 15685:2012)			1
Mwcnts_1_np_syn	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Mwcnts_1_np_syn	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Mwcnts_1_np_syn	Daphnia Magna Acute Lethal Tests	D. Magna	Daphnia Magna	1
Mwcnts_1_np_syn	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Mwcnts_1_np_syn	Lysosomal Activity (neutral Red)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Mwcnts_1_np_syn	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Mwcnts_1_np_syn	Metabolic Activity (alamarblue)	RtI-w1	Rainbow Trout Liver Cells-waterloo 1	1
Na2wo4 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Na2wo4 Salt (ion Control)	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Na2wo4 Salt (ion Control)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Na2wo4 Salt (ion Control)	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Na2wo4 Salt (ion Control)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Na2wo4 Salt (ion Control)	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Nm-403	Potential Ammonium Oxidation (iso 15685:2012)			1
Org P. Red254	Potential Ammonium Oxidation (iso 15685:2012)			1
Orgpig (irgazin)	Springtails Tests	F Candida	Folsomia Candida	1
Pigment_1_np_syn	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Pigment_1_np_syn	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Pigment_1_np_syn	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Pigment_1_np_syn (orgpig Red254)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Pigment_1_np_syn (orgpig Red254)	Daphnia Magna Acute Lethal Tests	D. Magna	Daphnia Magna	1
Pigment_1_np_syn (orgpig Red254)	Lymanea Stagnalis Acute Lethal Tests	L. Stagnalis	Lymnaea Stagnalis	1
Pigment_1_np_syn (orgpig Red254)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Pigment_1_np_syn (orgpig Red254)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Pigred101 (fe2o3_1_np_syn)	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Pigred101 (fe2o3_1_np_syn)	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Pigred101 (fe2o3_1_np_syn)	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Ref 17206	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref 17206	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref 17206	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref 17623	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref 17623	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref 17623	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Ref 17623	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Ref17206	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Ref17206	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Ref17206	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Ref17623	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1

Substance Name	End Point	Cell Type	Cell Type Desc	Count
Ref17623	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Wcco	Oecd Guideline 209			1
Wcco	Potential Ammonium Oxidation (iso 15685:2012)			2
Wcco	Springtails Tests	F Candida	Folsomia Candida	1
Wcco_1_np_syn	Cell Membrane Integrity (cfda-am)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Wcco_1_np_syn	Cell Membrane Integrity (cfda-am)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Wcco_1_np_syn	Daphnia Magna Acute Lethal Tests	D. Magna	Daphnia Magna	1
Wcco_1_np_syn	Lysosomal Activity (neutral Red)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Wcco_1_np_syn	Lysosomal Activity (neutral Red)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1
Wcco_1_np_syn	Metabolic Activity (alamarblue)	Clc	Carp (cyprinus Carpio) Leukocyte Cell Line	1
Wcco_1_np_syn	Metabolic Activity (alamarblue)	Rtl-w1	Rainbow Trout Liver Cells-waterloo 1	1

WP5: Occupational and consumer exposure

NOAA inhalation, dermal and dermal-to-oral exposure measurements, process-specific release potentials and exposure protection measures data received from WP5 giving total of 96 measurements. The data have been exported from NECID database which was used by the partners to capture the data originally and included in the SUN Operational Database. Table 4 summarises the available exposure measurement data.

Table 4: Summary of WP5 exposure scenarios

Product Name	Activity	Source Domain	Sampling Specification	Count
Carbon nanotubes	Extruder	Hot processes	Personal	5
Carbon nanotubes	Extruder	Hot processes	Static	2

Product Name	Activity	Source Domain	Sampling Specification	Count
Carbon nanotubes	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Personal	15
Carbon nanotubes	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Static	7
Carbon nanotubes	Other solids	Hot processes		2
Carbon nanotubes	Other solids	Hot processes	Personal	16
Carbon nanotubes	Other solids	Hot processes	Static	2
Carbon nanotubes	Transfer of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Personal	22
Carbon nanotubes	Transfer of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Static	14
Catalyst	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Personal	1
Catalyst	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Static	2
Catalyst	Transfer of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Personal	1
Catalyst	Transfer of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Static	1
metal-hydroxides	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Personal	2
metal-hydroxides	Falling of powders or granules	Handling and transfer of bulk manufactured nanomaterial powders	Static	3

WP6: In-vitro toxicology data

Table 5 summarises the in-vitro data returns which have been catalogued and linked to the database, giving a current total of 17 tests and assay results datasets.

Substance Name	End Point	Cell Type	Assay Name	No of test result files
Cocl2	Fluorescence Measurement Of Extracellular Single Cell Dna (%) After Electrophoresis	СЗа	"fpg" Modified Alkaline Single Cell Gel Electrophoresis (scge) Or "comet" Assay	1
Copper Oxide	Fluorescence Measurement Of Viable Cells	СЗа	Alamar Blue	1
Copper Oxide Nanoparticles	Cytotoxicity	Raw264.7	Alamar Blue	1
Copper Oxide Nanoparticles	Short Term Inhalations Tudy (stis)		Toxicity Endpoints (test 1) As Well As Kinetic Endpoints/organ Burden Analysis (test 2)	3
Copper Oxide Nanoparticles (cuo)	Short Term Oral Tudy (stos)		Toxicity Endpoints	1
Coppercarbonate Nanoparticles (cuco3)	Short Term Oral Tudy (stos)		Toxicity Endpoints	1
Cuo	Fluorescence Measurement Of Extracellular Single Cell Dna (%) After Electrophoresis	C3a	"fpg" Modified Alkaline Single Cell Gel Electrophoresis (scge) Or "comet" Assay	1
Cuo Pei And Asc	Pulmonary Inflammatory After L Inhalation Of Nanomaterials			4
Cuo, Wcco	Fluorescence Measurement Of Extracellular Single Cell Dna (%) After Electrophoresis	СЗа	"fpg" Modified Alkaline Single Cell Gel Electrophoresis (scge) Or "comet" Assay	1
Cuso4	Fluorescence Measurement Of Extracellular Single Cell Dna (%) After Electrophoresis	СЗа	"fpg" Modified Alkaline Single Cell Gel Electrophoresis (scge) Or "comet" Assay	1
Fe2o3 P Red 101	Cytotoxicity	Raw264.7	Alamar Blue	1
Fine Tungsten Carbide With Cobalt Binder	Cytotoxicity	Raw264.7	Alamar Blue	1
Fp7-sun Priority Pristine Nanomaterials	Luminex	RAW 264.7		1
Multi-walled Carbon Nanotubes	Cytotoxicity	Raw264.7	Alamar Blue	2

 Table 5: Summary of WP 6 test results returned and added to the database

Substance Name	End Point	Cell Type	Assay Name	No of test result files
Orgp Red 254	Cytotoxicity	Raw264.7	Alamar Blue	1
Silicon Dioxide	Cytotoxicity	Raw264.7	Alamar Blue	1
Tio2(in Acid Water)	Cytotoxicity	Raw264.7	Alamar Blue	1
Tio2(in Monopropylene Glycol)	Cytotoxicity	Raw264.7	Alamar Blue	1
Tungsten Carbide - Cobalt	Fluorescence Measurement Of Viable Cells	СЗа	Alamar Blue	1
Wcco	Fluorescence Measurement Of Extracellular Single Cell Dna (%) After Electrophoresis	СЗа	"fpg" Modified Alkaline Single Cell Gel Electrophoresis (scge) Or "comet" Assay	1

WP6: In-vivo toxicology data

Table 6 summarises the in-vitro data returns which have been catalogued and linked to the database, giving a current total of 9 tests and assay results datasets.

Substance Name	End Point	Animal Name	Δnimal Δge	No of test result files
Copper Oxide Nanoparticles	Short Term Inhalations Tudy (stis)	Wistar Rats	10 Weeks In Experiment	3
Copper Oxide Nanoparticles (cuo)	Short Term Oral Tudy (stos)	Wistar Rats Rjhan:wi	9-10 Weeks At Start Of Experiment	1
Coppercarbonate Nanoparticles (cuco3)	Short Term Oral Tudy (stos)	Wistar Rats Rjhan:wi	9-10 Weeks At Start Of Experiment	1
Cuo Pei And Asc	Pulmonary Inflammatory After L Inhalation Of Nanomaterials	Rjhan:wi	10 Weeks (exposures)	4

 Table 6: Summary of WP6 In-vivo test results returned and added to the database

WP7: Safe production, handling and disposal

For WP7 a data set from the electrochemical tests performed on Cu2 and CuO NPs added saline buffers and biological media and summary of relevant results of Phys-Chem characterization, for (eco)Tox tests is linked to the operational database as in figure 9.

A	B	С	D	E	F	G	Н	1	J	K	L	M	N
test	code	Capping agen	Disaggregation	Syn media			caratterizzazior	he			tox in	vitro test results	
condition					DLS	3	Dissolution 1h	Dissolution 24h	pН	BMD20	IC50	LC50 95h	EC50 (30 days)
					Z-Ave (nm)	ZP (mV	Cu ²⁺ /Cu _{tet} (%	Cu ²⁺ /Cu _{tet} (%)]				
	CuO_24	Pristine	US	water	330	34.9			6.4				
	CuO_91	Pristine	BM	water	301	35			6.8				
MilliQ	CuO_11	PEI	BM	water	222	49.9			7.3				
Water	CuO_11	ASC	BM	water	697	-8.3			6.4				
100mg	CuO_10	(CIT	BM	buffer PO4	226	-26.6			7.9				
CulL		Pristine	BM	buffer PO4	1093	-9.1	0.43	0.23					
(37 °C for	CuO_10		BM	buffer PO4	368	-18	2.31	2.47					
dissolution	CuO_10	(PVP	BM	buffer PO4	797	-8.1	0.98	0.29					
)	CuO_10		BM	buffer PO4	247	28.3	2.09	3.56					
	CuO_10		BM	buffer PO4	122	-17.4	2.6	2.49					
		CuCO3	BM	buffer PO4	180.57	35.5	0.21	0.28	5.9				
		Pristine		added from powder						✓ HWU (Stone)			
MEM		Pristine	BM	buffer PO4	47.2	-10.1	62.21	74.86	8.2	✓ HWU (Stone)			
100mg Cu/L	CuO_10	1 CIT	вм	buffer PO4	89.5	-10.5	43.39	69.04	8.2	✓ HWU (Stone)			
(37 °C for	CuO_10		BM	buffer PO4	43.8	-10.1	50.66	42.51		✓ HWU (Stone)			
dissolution			BM	buffer PO4	46.1	-10.5	34.97	53.8					
1	CuO_10		BM	buffer PO4	51.6	-9.5	42.88	60.16					
	040_10		BM	buffer PO4	0.0	0.0	42.00	00.10	0.2	• Hwo (otone)			
DMEM	LCUO 10	Pristine	BM	buffer PO4	55.1	-8.2	66.9	84.26	8.1	✓ KI (Bengt)	✓ KI (Bengt)		
50mg Cu/L	CuO_10		BM	buffer PO4	37.4	-9.7	67.21	83.64			✓ KI (Bengt)		
(37 °C for	CuO_10		BM	buffer PO4	52.9	-9.4	61.97	82.51			✓ KI (Bengt)		
dissolution			BM	buffer PO4	44.6	-10.1	61.97	82.51			✓ KI (Bengt)		
)	CuO_10		BM	buffer PO4	72.8	-9.2	63.14	81.74			✓ KI (Bengt)		
	CuSO,			water								✓ HWU (Ricottone)	
OECD		Pristine		added from powder								✓ HWU (Ricottone)	✓ HWU (Ricottone)
50mg Cu/L		Pristine	вм	buffer PO4	2364	-3.37	0.03	0.09	7.1			✓ HWU (Ricottone)	
(25 °C for	CuO_10	1 CIT	BM	buffer PO4	1615	-10.6	1.28	1.37	6.4				
dissolution			BM	buffer PO4	2098	-6.69		0.01	7.3			✓ HWU (Ricottone)	✓ HWU (Ricottone
)	CuO_10	PEI	BM	buffer PO4	284	22.35	2.38	2.58	7.7				
	CuO_10	ASC	BM	buffer PO4	1719	-9.52	0.95	0.9	6.7			✓ HWU (Ricottone)	✓ HWU (Ricottone)
AF∀	CuO_10	Pristine	BM	buffer PO4	4244.5	-3.5	0	0.25					
100mg	CuO_10	¢CIT	BM	buffer PO4	3890	-3.58	2.52	2.05					
CulL	CuO_10	(PVP	BM	buffer PO4	5964.5	1.64	0.02	0.1					
(25 °C for	CuO_10	PEI	BM	buffer PO4	2443.5	20.9	6.88	6.26					
dissolution	CuO_10	ASC	BM	buffer PO4	2142	-8.08	1.2	0.71					
AMW	CuO_10	Pristine	BM	buffer PO4	4279.5	7.61	0.04	0.27					
100mg	CuO_10	CIT	BM	buffer PO4	3395.5	4.53	3.07	2.41					
CulL	CuO_10		BM	buffer PO4	5077.5	6.48	0.06	0.12					
(25 °C for	CuO_10	PEI	BM	buffer PO4	4918.5	10.08	3.15	7.41					

Figure 9: Summary of results of Phys-Chem characterization, for (eco) Tox

WP 4 OMICS Datasets

Given the voluminous nature of OMICS results files these tests stored their OMICS data in industry standard fashion in recognised formats in appropriate OMICS public repositories. These can be made accessible to permitted users. The NCBI repository is used to suitably catalogue and publish the Folsomia candida genome sequence datasets. This strategy is clearly more practical than attempting to attach huge volumes of data directly to the SUN Operational or the eNanoMapper databases, neither of which have the capacity or facilities to manage such voluminous datasets. In liaison with the omics data co-ordinator, we have obtained summary descriptive information and uploaded this to the Operational Database to provide basic information describing the datasets which are in turn hyperlinked to the appropriate project page and OMICS dataset resources in the on-line repository. This is demonstrated in figure 10.

Folsomia cand	lida strain:VU population Genome sequencing and assembly
Accession	PRJNA299291
Data Type	Genome sequencing and assembly
Scope	Monoisolate
Submission	Registration date: 20-Oct-2015
NCBI Portal	https://www.ncbi.nlm.nih.gov/bioproject/PRJNA299291/
UV Portal	http://collembolomics.nl/folsomia/portal/data/
Organism	Folsomia candida[Taxonomy ID: 158441] Eukaryota; Metazoa; Ecdysozoa; Arthropoda; Hexapoda; Collembola; Collembola; Entomobryomorpha Isotomoidea; Isotomidae; Proisotominae; Folsomia; Folsomia candida
Enchytraeus c	rypticus strain:VU strain Transcriptome or Gene expression
Accession	PRJNA207507
Data Type	Transcriptome or Gene expression
Scope	Multiisolate
Submission	Registration date: 7-Jun-2013
NCBI Portal	https://www.ncbi.nlm.nih.gov/bioproject/PRJNA207507/
Organism	Enchytraeus crypticus[Taxonomy ID: 913645] Eukaryota; Metazoa; Lophotrochozoa; Annelida; Clitellata; Oligochaeta; Haplotaxida; Tubificina; Enchytraeidae; Enchytraeus; Enchytraeus crypticus

Figure 10: external links to OMICS repositories

Folsomia candida genome sequence and related information can be found under Bioproject: PRJNA299291

https://www.ncbi.nlm.nih.gov/bioproject/PRJNA299291/

http://collembolomics.nl/folsomia/portal/data/

Files	Description
Fcan01.stats	Folsomia candida genome and annotation statistics
Fcan01_annotation.tsv	Folsomia candida annotation summary
Fcan01_proteins.fa.gz	Folsomia candida proteins
Fcan01_transcripts.fa.gz	Folsomia candida transcripts
Fcan01_assembly.fa.gz	Folsomia candida Assembly
Fcan01_genes.gff.gz	Folsomia candida genes (GFF)
Fcan01_repeats.gff.gz	Folsomia candida Repetitive sequences (GFF)
Fcan01_repeats.txt	Folsomia candida Repetitive sequences summary
Fcan01_swissprot.blastout	Folsomia candida blast results against SwissProt database
Fcan01_trembl.blastout	Folsomia candida blast results against TrEMBL database
Fcan01_interpro.tsv	Folsomia candida InterProScan results (TSV)
Fcan01_interpro.gff3	Folsomia candida InterProScan results (GFF)
Fcan01_mapping.bam	Folsomia candida Bowtie2 mapping (Illumina)
Fcan01_pacbio.bam	Folsomia candida mapping (PacBio)
Fcan01_VAR_filtered.vcf.gz	Folsomia candida variants (SNP/INDELs)
SRR935329_hisat2.bam	Folsomia candida HISAT2 transcriptome mapping (SRR935329)
SRR921597_hisat2.bam	Folsomia candida HISAT2 transcriptome mapping (SRR921597)

Transcript sequences used for bisulfite sequencing in Enchytraeus crypticus are deposited under: PRJNA207507

https://www.ncbi.nlm.nih.gov/bioproject/PRJNA207507/

8. Sharing of the operational SUN database

Notwithstanding other potential developments for data sharing in the near future with the eNanoMapper database via other projects as described in earlier sections and further below, it is anticipated that in future (as in other earlier projects, e.g. ENPRA and MARINA) the SUN operational database may be supplied to other interested third parties, subject to approval by the project coordinator and consortium and any appropriate confidentiality or other sharing agreements being made. This will be done with secure transit arrangements made in advance with any recipient, e.g. the files are only made available for transfer via an encrypted file format (in an encrypted zip file). In order to facilitate its use by others the database contains brief introductory information, available from the main menu, with contact details to obtain more information from WP1. In addition, introductory instructions for database users are also provided in a covering document.

9. Coordination activities with other projects

The SUN partners in WP1.2, initially following various achievements related to Nano-EHS physchem and toxicology data management, template development, and modelling have in recent years been closely involved in developments to harmonise and standardise the data, databases and methods to enhance the sharing and exchange of data in this field. This has been through work on FP7, and more lately H2020, projects, in the Nano-EHS community primarily via the Nano Safety Cluster (NSC), and beyond - e.g. via US-EU-CoR collaboration efforts. Such efforts aim to develop materials and methods so that Nano EHS project data will be able to conform as far as possible with emerging data standards for nanomaterials and Nano toxicology research, and associated database and ontology developments in the growing field of Nano Informatics. WP 1.2 partners have consistently been keen participants and significant contributors to these efforts in recent years.

We are also highly aware of and have been very actively and closely involved in recent years with the on-going collaborations and research – via connections with the NSC-WG4 (Database WG) and its active players in this field, via eNanoMapper members in the WG and the eNanoMapper coordinator via the Cluster and the US-EU CoR. We have also had other ongoing interactions on the exchange and update of our existing templates in the MODENA-COST action, and with other contemporary projects that have been examining: harmonisation, minimum information and data-definition standards for nanomaterials (phys-chem); ontologies; Nano-database design; and associated toxicology and exposure data formats, templates and handling and exchange processes. These projects include NanoPuzzles, MODERN, ongoing ISA-Tab-Nano developments, as well as in the context of information gathering and management the execution of a Nano-EHS database mapping exercise in PROSAFE. Naturally experiences and information flow to and from each of these research and development areas and projects in which we have been involved, including SUN, in mutually beneficial ways through cooperation, collaboration and sharing of knowledge and resources.

10. Coordination activities with eNanoMapper

WP1 T1.2 has been well aware of the FP7 eNanoMapper project and has positively interacted with it from first contact in 2014. ENanoMapper is developing a computational infrastructure for the management of toxicological data on engineered nanomaterials (ENMs) based on open standards, the development and use of appropriate ontologies and an interoperable design to enable a more effective, integrated approach to information sharing in nanotechnology EHS research. It has sought collaborators like SUN who are managing data in these fields. It is noted that some of the interactions and discussions we have had also had useful cross-over to the NANOSOLUTIONS project, as these also involved WP1 data management personnel contemporaneously to the SUN work.

Following initial contact we provided and discussed views on the "state of the art" in this field, in relation to the needs and a formal requirements analysis for nano-EHS data generators,

curators, managers and end users, with the eNanoMapper team. This was later followed-up with further interaction in a more in-depth interview (autumn 2014) and subsequently in many follow-up discussions with the eNanoMapper Project Coordinator and other eNanoMapper staff (principally EW and NJ) on ontology and database aspects many times over the last three years, particularly the last 18 months. Several similar and related discussions were also mediated by the US-EU-CoR, to which we also contributed.

SUN WP1 and eNanoMapper agreed interactions to help test developments, data formats and processes, with the aim of ultimately supplying (SUN) data to the idealised nano-EHS database when both were suitable for such an exchange. Initial priorities in this regard were for the exchange of phys-chem and (in-vitro) toxicology templates, and our involvement has undoubtedly contributed substantially to the data upload and exchange developments seen in eNanoMapper developments to date. We still aim to exploit these further, given a suitable eNanoMapper implementation for SUN being set up, and we are aware that hands-on training and guidance on their use has recently been made available.

We have interacted with eNanoMapper to develop, explore and assist in testing ideas, tools and solutions being developed, primarily in the areas of Nano-tox data, and to be able to access real case studies with toxicology and eco-toxicology datasets. We have had many positive interactions and discussion with the lead eNanoMapper database developer (NJ), particularly regarding the use and increasing harmonisation of data templates and formats. We had earlier anticipated making use in SUN of a far better developed and user friendly ISA-TAB-Nano based format and process for nano-EHS toxicology test data (and its related metadata, ontology features etc.), as a test of eNanoMapper developments. However, this has proven a far harder model to implement in practice, with the preference pro-tem to use our IOM or JRC derived templates for data capture. The ISA-TAB-Nano is only recently meditated in the eNanoMapper implementation as an output format, and essentially is without end-user friendly interface facilities for data-entry, and we have not been in a position to be able "retro-fit" such developments into the SUN repository

Related developments by eNanoMapper in this area to which we have contributed greatly (via our collaboration on nano-tox templates), have progressed significantly in eNanoMapper. We currently understand that further work to progress various aspects of this will continue and that this is now to be undertaken within the NanoReg2 project, in which members of SUN WP1 will participate as part of the "data solutions team". It is proposed that instances of eNanoMapper database will be implemented as receptacles for data from other earlier projects, which will include SUN. We have also agreed with eNanoMapper (autumn 2016) that we will provide (at least a sample of) ecotox data in our templates (which ultimately are derived from our in-vitro tox templates) for testing and incorporation into the eNanoMapper database model.

In addition to the above discussions and developments in the integration of nano-exposure data into eNanoMapper have taken place within the last 12-18 months, involving initially eNanoMapper, SUN-WP1 and WP5 (exposure), and later also others from the NSC WG4 (database) and WG6 (exposure) and the NECID (Nano Exposure and Contextual Information Database) initiative. This has led to the integration of exposure data as an additional data

domain into the eNanoMapper model, and the extension of the eNanoMapper ontology for nano-exposure data, with the potential to integrate exposure data, (and ultimately full NECID exposure datasets), into eNanoMapper. We are aware that this has not been implemented in the enanoMapper database software yet but at a suitable point we aim to help test this by populating the implementation with SUN generated exposure data. Besides the NECID exposure data aspects we have also discussed with eNanoMapper the potential for integrating the IOM Nano Exposure Scenario Library approach (with pre-formatted templates and reports), as implemented earlier in MARINA and referenced in SUN, for more general exposure data management and this will progress in subsequent projects.

Whilst we have been able to collaborate and contribute to developments for the several data types above, despite the advances made to date the eNanoMapper database has of course needed to concentrate on certain data domains, so it cannot yet readily or simply accommodate all types of Nano-EHS data, including SUN data which it has not yet been designed or implemented to include. The prime example for SUN in this regard is in Environmental Release, Fate and Exposure data (WP3) and related nanomaterial lifecycle issues. Hence via WP1 the SUN coordinator has more recently initiated a new working group on this area (being mediated via NSC WG4 (databases)) to discuss and explore the possibilities for harmonising the recording and storage of such Release, Fate and Exposure data, and their future incorporation into an instance of eNanoMapper. Once implemented this would lead to the upload of such SUN data. Initially the working group principally includes SUN partners from WP1, and WP3, and eNanoMapper.

Noting formal presentations of aspects of all of the above work and collaboration, from WP1.2 IOM presented the database and management work of SUN (and other related efforts) in a presentation at a 2 day meeting on data harmonisation and knowledge infrastructure and framework for nano-EHS, (26/01/16, Brussels). Also IOM from WP1 was on the organising committee of the Nano-EHS EU-US Bilateral Workshops, 24-25 Oct, Rheinfelden, Germany, and presented on "Towards nano-ehs data harmonisation - template use experiences in recent FP7 projects and related initiatives". The major contribution to developments from the SUN project (and others, including the various interactions noted above) was highlighted and gratefully acknowledged in the talk by the presenter. This also led to our connection to the currently ongoing development of a "Nano Informatics Roadmap", and our being invited to be part of the Task Group to write it, in a collaborative effort between the NSC and US-EU-CoR. Again credit must be given to efforts and work on SUN that has helped enable our participation in this.

We will naturally continue to share and contribute to new and on-going developments in templates, other data curation materials and methods, database design and implementation, metadata and ontologies - more generally, participating in the expanding field of Nano Informatics development) with other similar H2020 projects, COST initiatives, eNanoMapper and other NSC WGs where appropriate. We intend to make as much of the SUN data available as possible to eNanoMapper for upload, either before conclusion of the project, or if that has been exceeded, then continuing under the auspices of one of the other ongoing developments

including NanoReg2 (<u>http://www.nanoreg2.eu</u>) or CaLIBRAte (http://www.nanocalibrate.eu/home), for example.

11. Deviations from the Work plan

There are no deviations from the work plan with regard to database design or implementation in WP1. In addition to the original DoW we have as requested also actively contributed to wider developments in the field of Nano-EHS database developments, the NSC UE-EU-CoR, and interactions with eNanoMapper, and SUN resources contributed to this. As noted in the relevant sections above, due to problems and delays elsewhere in the project it is suggested that some small portions of outstanding data may still be returned to WP1, and with best endeavours WP1.2 will add this to the operational database.

12. Performance of the partners

Partners in WP1 have fulfilled their tasks in satisfactory time and quality.

13. Conclusions

Task 1.2 has successfully accomplished the design, implementation and population of the SUN data repository database. An extensive exercise was been carried out with Sun project partners to develop data templates and data collection, and to procure, collate and curate the scientific project data into a flexible and user-friendly operational database. This is immediately available from WP1, although at this final juncture we still await some minor additions to the datasets from partners due to delays out-with WP1's control. Thus the final (latest possible) updated SUN database will be made available to partners from the site Sun.iom-world.co.uk.

In addition we have significantly contributed to the wider development and harmonisation of Nano-EHS data, databases and nanoinformatics more generally through our interactions with the enanoMapper project itself, the NSC Database Working Group, and other related initiatives, which have, at least in part, been resourced through the SUN project.

We anticipated sharing SUN data more generally early on in the task, and as the work evolved, providing data to be uploaded to an instance of the "final" eNanoMapper database. We will make this data available, though as mentioned data sharing permissions, embargos etc. will need to be formalised and observed at appropriate levels in the short term. To advance this, we are currently involved in further related developments, having been contacted by the NANOREG2 and CaLIBRAte projects, aiming to supply them with final data from projects that we have data-managed (e.g. SUN, MARINA, NANOSOLUTIONS). From our discussions with these initiatives it is anticipated that effectively an instance of the eNanoMapper database, (or possibly a suitably partitioned and secured single instance) will be implemented to hold the

data from each donating project, including SUN, with selective approvals and permissions for use being managed by the database. As such the SUN instance would provide the ideal eNanoMapper formatted repository for the Sun data. We will in any case work collaboratively and cooperatively as we have done previously, to make sure that SUN data it is available for further use and exploitation by future projects and researchers.

More generally, as a further result of our work on SUN and related initiatives we will continue our community involvement to address issues around the continuing support, availability, accessibility and sustainability of FP7 and more recently H2020 data. (H2020 data now requires a mandatory Data Management Plan, and ideally the sustained availability of open data). As this has been well demonstrated by our involvement as part of the community, WP1 partners will continue to positively contribute to these developments and promote the availability and accessibility of project data through moves to establish and maintain the sustainability of such nano-EHS data resources. In this we will continue to acknowledge the contribution of the SUN project, in terms of experience gained and resources provided, to this and related developments in nanoinformatics.

Deliverable D1.2 "The SUN Project Database"

14. Appendices -key data template aspects of the operational database

Appendix 1: ENM characterisation data file

X 🖌 Y - (H - 1		SUN_PhyChem	_CharData_v4 - Microsoft E	xcel			
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1 SUN - characterisation of pri	stine nanomaterials for (eco)toxi	cological testing					î
	reat this as read-only & do not alter the		e, which during the proj	ect is only for			
3 limited distribution to SUN partners	s, or approved others subject to confid	lentiality discussions and ap	proval from project lead	ler Danail Hristozov (da	anail.hristozov@unive.it).		
4							
5 Do not alter or update the data in t	his edition; if you discover any errors, o	or anomalies, or have data to	be added, please info	m peter.ritchie@iom-v	vorld.org & shahzad.rash	id@iom-world.org (WP1)	
6							
	UN project as work progresses, in whi						
	an be used, allowing different data iten	ns and formats to be viewed	and used by partners i	n the course of work.			
9							
10 The key sheets and their contents							
11 WorkSheets: (Use the link to mov	ve directly to the particular sheet)						
12							
13 Samples List	Table 1. Details of each SUN sample, s			er.			
14 Primar Char Summary	Table 2. Summary of primary character		rtner.				
15 Primary Char Results Summary	Table 3. Summary of primary character						
16 TEM Primary Size Distribution	Table 4. Observation and measurement						
17 TEM Micrographs	Table 5. Representative TEM microgra		e distributions for selec	ed samples.			
18 Crystallite Size Phases	Table 3. Summary of primary character						
19 Dispersability Water Biological	Table 6. Water and biological medium			et by do not taking in acc	ount the peaks from the b	iological medium.	
20 <u>Z Potential</u>	Table 7: Z-potential results in UP wate		ilts at pH7.				
21 Photocatalytic Activity	Table 9. Photocatalytic activity data in						
22 Surface Area Pore Size	Table 10. Surface area and pore size re			ets (BJH: Barrett, Joyner	, and Halenda; AVG: Avera	ge Pore Size; DFT: Density I	Functional
23 Average Agglomeration No	Table 11. AAN for water dispersions an		I medium dispersions				
24 Surface Chemistry	Table 3. Summary of primary character						
25 <u>Structure</u>	Table 3. Summary of primary character						
26 Chemical Impurities	Table 3. Summary of primary character	rization results					
27							
28							
29							
30 31							
32 Index_Intro Samples_List	Primar Char Summary Primary Cha	r Results Summary TEM	Primary Size Distribution	TEM Micrographs	Crystallite Size Phases	Dispersability_Water_Biologica	I Isoelectric
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A1 👻 💿	<i>f</i> ∗ Ta	able 3. Summa	ry of primary of	characterization res	sults				
A	В	С	D	E	F	G	Н	l. I	J
Table 3. Summary of primary charact	arization re	culte							
Table 5. Summary of printery charact	Techniqu	Fe ₂ O ₃ _1_	CuO 1	MWCNT 1	SiO ₂ _1_	TiO ₂ acid	TiO ₂ monopropylene	WC+Co 1	OrgPig_1_
	e	NP_PROD	NP_PROD	NP_PROD	NP_PROD	water_1_ NP PROD	glycol_1_ NP_PROD	NP_PROD	NP_PROD
Primary size distribution Min- Max (average) Mode (1st quartile 3rd quartile) [nm]	тем	11-112 (37) 32 (2843)	3-35 (12) 10 (9.214)	Ø: 4-16 (8) 7.4 (6.79.2) L: 575-3462 (1543)	3-27 (11) 9.5 (814)	1-15 (4) 3.2 (2.94.4)	1-5 (3) 2.8 (2.53.5)	23-1446 (170) 48 (69280)	14-151 (43) 26.3 (29.849
Shape	TEM	Irregular rounded particles	Semi-spherical particles	1020 (9201800) Bent and partially entangled multiwalled	Irregular polyhedrons and some spherical particles	Very small irregular polyhedrons and some spherical particles	Very small irregular polyhedrons	Irregular polyhedral particles and some semi- spherical with	Irregular polyhedrons a some small se spherical parti
Average crystallite size [nm]	XRD	40	9.3	Not measurable	(JRC-IHCP) Synthetic amorphous silicon dioxide, impurities of Bohemite	18 (43%) 6.8 (57%)	10.6 (14%) 3.2 (86%)	15.4	No database available
Crystallite phases (%)	XRD	Hematite 100%	Tenorite 100%	(Nanogenotox) carbon nanotubes	(JRC-IHCP) 22 nm	Main phases: Brookite and rutile; Third phase: a salt or an oxide	Mix of anatase, rutile and brookite	Tungsten carbide 100%	No database available
Dispersability in water: D ₃₀ [nm]; average agglomeration number (AAN)	DLS	177.3±6.6; 39	139.5±4.6; 346	(JRC-IHCP) 175.9±4.5; 2419	(ENPRA) 216; 6036	85.9±1.3; 19411	82.1±4.8; 25117	182.8±21.5; 31	137.3±4.6 41
Dispersability in modified MEM provided by the Heriot-Watt University: D ₁₀ [nm]; average agglomeration	DLS	148.2±2.2; 23	85.2±2.7; 77	Not available	Not available	60.0±2.6; 6592	Unstable sample	315±18; 159	84.4±4.5; 9
Z-potential in UP water [mV]	ELS	+32.0±0.7	+28.1±0.6	Unstable sample	-37.6±0.8	+39.3±1.1	+32.9±2.2	+7.1±0.5	-20.8±1.3
Isoelectric point [pH]	ELS	9.7	10.3	Unstable sample	1.8	In progress	In progress	<2	2.1
Photocatalysis: photon efficiency [unitless]	Methylen e blue degradati on	Not measurable (pigment)	1.5×10 ⁴	9.5×10°	1.3×10 ⁴	2.4×10 ⁻⁵	2.4×10 ⁻⁵	6.7×10 ⁴	Not measural (pigment)
Specific Surface Area [m² g⁻³]	BET	22.6±0.1 30 (from producer)	47.0±1.7	From other EU project 339.3 ± 17.3	From other EU project 190.5 ± 4.0	Sample degradation during degassing	Sample degradation during degassing	6.6±0.4	94 (from produ
Pore sizes [nm]	BET	65 (from producer	13.5±1.6 (SUH) 23.0±0.9 (AVC)	Not available	Not available	Sample degradation during degassing	Sample degradation during degassing	Non porous	80, 200 to 2×1 (from produc
Surface chemistry [atomic fraction]	XPS	C 50.7 O 33.7 Fe 15.6 (from producer)	Cu = 0.46±0.05 0 = 0.47±0.05 C= 0.07±0.01	Not available	(JRC-IHCP) O (72.1 at%), Si (25.0 at%) and C (2.9 at%) due to surface	In progress	In progress	Co=0.08±0.01 W=0.05±0.01 O=0.31±0.03 C=0.56±0.05	C 77.1 O 10.9 N 5.9 Cl 6.1

Appendix 2: Characterisation data summary

Appendix 3: In-vitro test method description form

SUN TEST METHOD DESCRIPTION FORM

INFORMATION ON TEST METHOD AND PARTNER						
Name of test method Cell viability: Alamar blue (resazurin) assay						
Acronym of test method	Citotoxicity: Alamar blue assay					
	Organisation Name	WP ID	Partner ID			
Proposer - Organisation	Heriot Watt University	WP6	25-HWU			
	Heriot Watt University – Riccarton Campus					
	School of Life Sciences					
Postal address	John Muir Building					
	EH14 4AS					
	ик					
Name of contact person	Daniele Pantano					
Tel. no. of contact person	+					
Fax no. of contact person	+					
e-mail of contact person	dp163@hw.ac.uk					

WP	11 - STUDY DATABASE ADMIN USE ONLY
Received (Name/Date)	
Related data record files	
- (Excel Templates)	
Related NSNP characterisation	
file(s)	
Follow-up?	
DB Entry Notes	
Check completion (Name/Date)	
Document category	
Document ID	
Record ID	

Please be sure to complete all relevant sections as fully as possible

1. Describe the scientific and technical basis of the test method					
 What biological/cellular model is the method based on? 					
C3A (ATCC [®] CRL-10741 [™]), derivative of Hep G2 (ATCC HB-8065)					
 What biological endpoints/responses does this method address? 					
Cell viability (mitochondrial enzyme activity)					
What specific mechanisms associated with the biological response are targeted?					
Assay measures the conversion of the oxidized form of Alamar Blue to the reduced form by mithocondrial enzyme activity by accepting electrons from NADPH, FADH, FMNH, NADH as well as from the cytochromes.					
What methods/techniques are used for endpoint/response determination?					
Conversion of resazurin (non-fluorescent indicator dye) to resorufin (bright red- fluorescent) via the reduction reactions of metabolically active cells. The redox reaction is accompanied by a shift in colour of the medium from indingo blue to fluorescent pink. The amount of fluorescence produced is proportional to the number of living cells.					
 Was the method originally developed for a particular applicability domain (e.g. testing of a certain class of chemical)? 					
N/A					
Are there potential technical limitations of this method for testing nanomaterials?					
Some nanoparticles interfere with the assay (interference test for each material is done during the assay)					

2.	Describe the role of the method in context of hazard assessment for human health
•	How should the information/results derived from the method be interpreted in relation to an in vivo response/endpoint?
	N/A
•	How could the information derived from the method be used to refine, reduce or replace an animal test, as specified in recognised testing standards and guidelines (e.g. OECD Test Guidelines)?

The experiment gives a preliminary idea of the range of toxicity of the nanomaterial, this would help in planning the *in vivo* exposures both reducing sensibly the

amount of animals involved in the experiments and avoiding to use too high amount of NMs inducing obvious side effects in the models.

What are specific limitations of this test in terms of predicting hazard to human health?

Cell lines give a partial response in term of total toxic effect compared to an organisms because of the lack cellular-cellular specific interactions and tissue 3D structure with his histological characteristics.

 What other tests (in vitro, in vivo, in silico) would be required to compliment this method to give a better assessment of hazard, or prediction of an in vivo response?

It is always a good procedure to include other cellular models that could be representative of different route of exposure/organs exposed. After that preliminary analysis, an *in vivo* confirmation is due for the lack in predictivity of the cellular models.

3. Describe the Standard Operating Procedure (SOP)

The SOP should be complete, self-contained and well presented. It should be described in sufficient detail to enable the method to be reliably and efficiently transferred between labs. The SOP should cover the following points:

- Details of the organisation who drafted the SOP and contact person
- Short description of the method and its scientific and technical basis
- Description of positive/negative controls
- Materials
 - Biological model (cells)
 - Technical equipment
 - Reagents, media and sera
- Preparation of media, solutions and controls
- · Methods for cell maintenance and culturing
- · Preparation of test substances
- Testing procedure
 - Plate format
 - Treatment of model/cells with test substance
 - Quality checks
 - Endpoint measurement
- Data analysis
- Test acceptance criteria
- Results reporting requirements
- Additional information
- References

Please attach the SOP as a separate document if appropriate, and / or give full link reference to the document on Project website version – please include version number



(if	app) included
W	P6-Toxicology and Human Health Risk FP-7 SUN Project
Att	tached as separate document in e-mail – eg also available on website at
4.	Performance assessment of the method
	Describe the scope of the performance assessment study and how it was undertaken.
In	vitro screening method
I	The second guided
	What test substances were used for assessment purposes and what was the basis for
l.	their selection?
	Copper oxide nanoparticles, fine tungsten carbide with cobalt binder nanoparticles.
•	What were the specific criteria used to judge/describe test method performance?
	Statistical analysis using Benchmark doses approach
	Was the study conducted under GLP, and/or did it adhere to a recognised quality system?
Ye	
"	
	What was the reliability of the assay in terms of intra-lab and inter-lab reproducibility
1	
	Low standard deviation measured within three different experiments. No inter-lab testing.
•	If the performance assessment included the comparison of in vitro and in vivo data, how
	well did the in vitro results correlate with the in vivo outcome?
N//	A
1	

ADDITIONAL INFORMATION – Expand on to further pages if required

5. Pro	5. Provide key references to patents and/or relevant publications					
1						

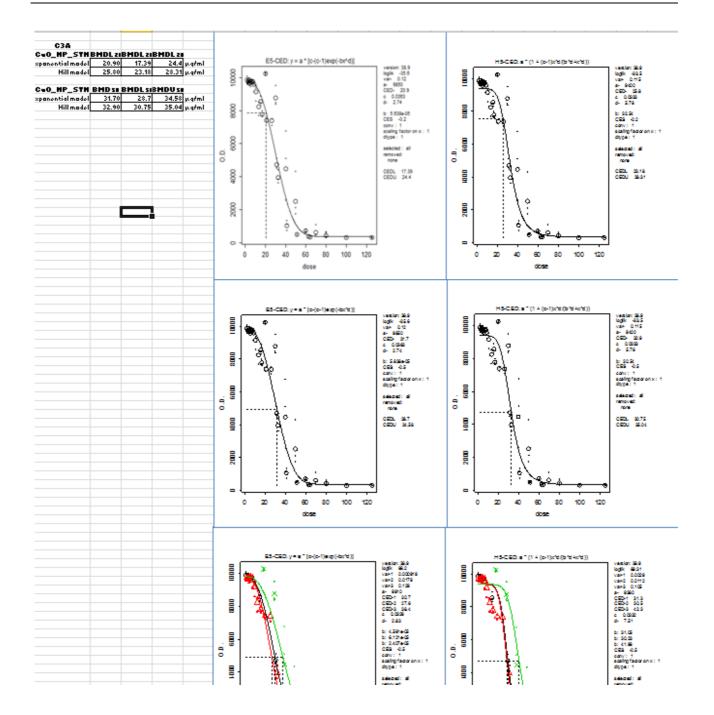
	ntify candidate laboratories that are sufficiently experienced to participate in a nal prevalidation or validation study
1	N/A

 Add here any further information or particular attributes of this Assay/Test and associated datasets that will assist other WPs, or a potential third party making use of

Appendix 4: In-vitro tests data collection template

TEST CONDITIONS	Please compl	ete the detai	Is below as far	as pose	sible for e				
In-Vitro Testing	While we must	While we must aim to standardise SUN toxicology data records							
	You may add additional items below where necessary for furth								
	in the notes ar	ea or adjacen	t to data tables,	add anno	otations w				
TEST and END POINT - GENERAL INFO									
SUN Vork Package:	WP6								
SUN Partner ID:	HVU								
Test facility - Lab name etc:	SLS - VP3 - Cell Cu	lture room							
Work conducted by:	Daniele Pantano		mail address:	dp163@hs	v.ac.uk				
Test / Assay End-Point short description:	Fluorescence meas	urement of viable	cells						
Assay:	Alamar Blue								
End-Point Outcome metric (ie % viability, %cell death etc):	0.D.								
SOP - Protocol Name:	CODA CUM Destant								
SUP - Protocol Name: Link to the SOP:	SOPs_SUN Project								
Test start date (dd/mm/qqqq):	Expt1: 03/05/14	Expt2: 10/05/14	Expt3: 17/05/14						
Test end date (dd/mm/gggg):	Expt1: 05/05/14	Expt2: 12/05/14	Expt3: 19/05/14						
TEST SUBSTANCE									
Substance name:	Copper Oxide								
Standard SUN Nanomaterial Code & Name:	CuO_NP_SYN								
Highest concentration used, inc units:	125	µg/ml							
rignest concentration used, inclutics:	120	pgrin							
DISPERSION									
Specify the standard dispersion protocol used:	see 'SOPs_SUNP	roject'							
(or otherwise specify the dispersion technique used)									
Dispersion agent?:	2% FBS in water								
Vere additives used? If so, specify which & concentration:	N	10.00							
Dispersed in cell culture medium?: Serum concentration (%):	only the subsequent 2%								
Serum concentration (%): Vas serum heat inactivated?:	2%. Y								
₩as serum near mactivated?:									
Aids used to disperse - Y / N:	onication-Bath:	Y	Sonication-tip	N	Vortezine				
Specify time-duration?:		, 16 mins.							
Energy (for sonication) :									
CELL LINE/TYPE									
Short-Name:	C3A	0 ODI 1071(79)	destruction of the D	ATOC:	(D. 0005)				
Full specific name (note any line variants or related IDs): Supplier:	HepG2/C3A (ATCC ATCC⊘	:∞ CRL-10741™),	derivative of Hep Gi	ZIATCCE	B-8065)				
CELL CULTURE CONDITIONS									
CELL COLTONE CONDITIONS									
Medium (Supplier/Lot No.):	Minimum Essential	Medium (MEM) -	Sigma-Aldrich Co.						
Serum (Supplier/Lot No.):	Fetal bovine serum		_						

expt 1		1	2	3	4	5	6	7	8	9	10	11	12
	A	В	C₀B	C₁B	C₂B	C₃B	C₄B	C₅B	C,B	C ₇ B	C₃B	C,B	В
	в	В	0.00	0.00	1.95	3.91	7.81	15.63	31.25	62.50	125.00	PC	В
	C	В	0.00	0.00	1.95	3.91	7.81	15.63	31.25	62.50	125.00	PC	В
		В	0.00	0.00	1.95	3.91	7.81	15.63	31.25	62.50	125.00	PC	В
	E	В											В
	F	В											В
	G	В											В
	Н	В	C ₁₀ B	C ₁₁ B	C ₁₂ B	C₁₃B	C₁₄B	C₁₅B	C ₁₆ B	C ₁₇ B	C₁₀B	PCB	В
expt 2		1	2	3	4	5	6	7	8	9	10	11	12
	A	В	C₀B	C₁B	C2B	C₃B	C₄B	C₅B	C₄B	C₁B	C₅B	C,B	В
	в	В	0.00	2.81	3.52	4.40	5.50	6.87	8.59	10.74	13.42	16.78	В
	С	В	0.00	2.81	3.52	4.40	5.50	6.87	8.59	10.74	13.42	16.78	В
	믹	B	0.00	2.81	3.52	4.40	5.50	6.87	8.59	10.74	13.42	16.78	B
	E	B	20.97	26.21	32.77	40.96	51.20	64.00	80.00	100.00	125.00	PC	В
	F	B	20.97	26.21	32.77	40.96	51.20	64.00	80.00	100.00	125.00	PC	B
	G	B	20.97	26.21	32.77	40.96	51.20	64.00	80.00	100.00	125.00	PC	В
	Н	В	C ₁₀ B	C ₁₁ B	C ₁₂ B	C₁₃B	C₁₄B	C ₁₅ B	C₁6B	C ₁₇ B	C₁₀B	PCB	В
expt 3		1	2	3	4	5	6	7	8	9	10	11	12
	A	В	C₀B	C₁B	C ₂ B	C₃B	C₄B	C₅B	C,B	C₁B	C₅B	C,B	В
	В	B	0.00	20.00	30.00	40.00	50.00	60.00	70.00	80.00	100.00	PC	В
	C	B	0.00	20.00	30.00	40.00	50.00	60.00	70.00	80.00	100.00	PC PC	В
	믿	B	0.00	20.00	30.00	40.00	50.00	60.00	70.00	80.00	100.00	PC	В
	E	B											B
	Ğ	B											B
	H	B	C ₁₀ B	C ₁₁ B	C ₁₂ B	C ₁₃ B	C₁₄B	C ₁₅ B	C ₁₆ B	C ₁₇ B	C ₁₈ B	PCB	B
		_	0100	0110	0120	0130	0140	0150	0160	0170	0180		
expt 1		1	2	3	4	5	6	7	8	9	10	11	12
	A	346.238	329.7	333.1	331	337.951	333.44	336.452	335.764	331.089	329.626	327.76	330.84
	в	351.29	9856	10118	10100	9844.1	9861.1	8894.4	5103.4	352.7	318.092	325.43	327.6
	C	352.07	9953	10064	9667	9931.5	9681.4	8303.9	4502	359.53	317.533	321.09	327.0
		367.31	9976	10035	9905	9875.7	9656.1	8484.2	4577.9	376.57	322.273	326.4	329.6
	E												
	F												
	G												
	н												
expt 2	+	1	2	3	4	5	6	7	8	9	10	11	12
•	A	347.09	339.41	352.93	347.09	374.32	357.64	359.54	352.14	359.74	341.03	361.11	341.54
	в		****	****	****	******	******	9818.45	9145.96	******	7699.21	*****	351.5
	С	357.91	****	****	****	******	******	******	******	9545.71	8533.66	*****	343.5
	D	378.38	****	****	****	9718.39	******	******	******	9361.55	8518.10	******	361.0
	E	365.37	****	****	****	747.38	446.49	323.43	314.98	287.88	283.46	315.65	358.0



	А	В	С	D	E F
1	copperoxide				
2	3				
3	0	1	1		
4	dose	O.D.	expt.		
5	1.95	10099.792	1		
6	1.95	9666.967	1		
7	1.95	9904.561	1		
8	3.91	9844.104	1		
9	3.91	9931.486	1		
10	3.91	9875.732	1		
11	7.81	9861.102	1		
12	7.81	9681.358	1		
13	7.81	9656.129	1		
14	15.62	8894.409	1		
15	15.62	8303.928	1		
16	15.62	8484.228	1		
17	31.25	5103.447	1		
18	31.25	4501.96	1		
19	31.25	4577.916	1		
20	62.5	352.697	1		
21	62.5	359.53	1		
22	62.5	376.572	1		
23	125	318.092	1		
24	125	317.533	1		
25	125	322.273	1		
26	2.8147	9718.707	2		
27	2.8147	9773.884	2		
28	2.8147	9735.42	2 2 2		
29	3.5184	9728.734	2		
30	3.5184	9669.268			
31	3.5184	9662.096	2		
14		t Conditions	Raw data	Raw da	ata for PROAST

Appendix 5: In-vivo tests data collection template

TEST CONDITIONS	Please comp	olete th	e details b	elov as	far as	possibl	e for ea
In-Vivo Template	While we aim to	to stan	dardise SUN	ia-vivo t	oxicolog	y data r	cords as
	You can add ac	ditional	items below	where as	cessary	for furth	er replica
	In the notes are	a or adj	acent to data	tables, a	dd anno	tations 1	rhere it s
n-Vivo - TEST and END POINT - GENERAL INFO							
SUN Work Package:	WP06						
SUN Partner ID:	Pxxs - llse						
Test facility - Lab name etc:	RIVM - GZB						
Work conducted by:	RIVM+contract research	arch animal	faciliy Intravacc	email ad	dress:		a@rivm.n
Test / Assay End-Point short description:	Short term Oral tudy	(2012)				lise.goser	2@rivm.nl
/Enter full description in the covering TMDF - assay description form)		131031					
pencertan deseription in the cortaining range assay deseription roam)	toxicity endpoints						
End-Point Outcome metric(s) (viability, death etc): /indicate how EP is derived)	gross pathology: lur Cu organ burdens: lu						
	D	UNL OT CO	(••
P - Protocol Name - ID (see project protocol ID list):	Research protocol S					port ICP-N	
(and or add path/link to protocol on SUN server.)	Z:/users/sun-project	waterialit	rotocols and Pro	scedures	Zinusersh:	un-project	uviaterial\l
Test start date (dd/mm/vvvv):	04/01/2016						
Test end date (dd/mm/yyyy):	29-04-2016						
TEST SUBSTANCE							
Substance name:	Coppercarbonate na	noparticles	; (CuCO3)				
CAS No:	12063-63-1						
Standard SUN Nanomaterial Code & Name:	CuCO3						
(See SUN Materials list)							
tandard Ref material (eq JRC) name/code where app:	not applicable						
Highest concentration used, inc units:	128	mg/kg Cu	ICO3.				
DISPERSION							
Specify the standard dispersion protocol used: /or otherwise specify the dispersion technique used)	Provided as liquid						
Dispersion agent:	Diluted Milli Q water						
Aids used to disperse - Y / N:	Sonication-Bath:	none	Sonication-t	NA	Yortezi	Y	Stirring
Specify time-duration?:							
Energy (for sonication) :							
			[
ANIMAL AND STRAIN ETC							
Hame:	Wistar rats RiHan:W	1					
Supplier:	Janvier Labs						
Ser:	male						
Age:	9-10 weeks at start o	, of experime	ant				
Average weight:	332 g at day 1 start o	xp					
TIMELINE							
The second damage of the second damage of the base	2						
Time points (hours - or specify any other units): Alter or add as necessary			l A Casus es Caler A	2.3.4.5	Pastionis -	94 kours -	fter first -
Mixer or add as hecessary	5 day consecutive ex	posare daŭ	o I davadel daŭ j	2-0-4-0	sectioning	24 nours a	rter rihare:
TREATMENT / DOSE CONCENTRATION							
Treatment dose range (mg/kg) animals exposed to CuO	group 1 O				group 5 16	group 6 8	group 7 4
NOTES - including any deviations from SOP; other obse Please include information on the handling or coding of missing or null		is etc. A	dd any inform	ation th	at will as	sist in t	e use ar

ST DATA	,	oxicity resu	1103											
CuCO3	2	3	4	5	6	7	8	9	10	11	12	13	14	
subst	inimal r	group n	lose mg/k	odų wt dau		y body wt	lung wt	adrenal	heart wt		themus	liver w	spleen	• kid
CuCO3	57	1	0	306	6	332	1.3922	0.0368	1.1767	3.4608	0.5282	12.9849		
CuCO3	58	1	0	327	6	357	1.6311	0.045	1.2399	3,4539	0.8288	14.2272	0.881	1 2
CuCO3	59	1	0	326	6	342	1.4147	0.0424	1.1564	3.4249	0.7524	13.0536	0.9549	
CuCO3	60	1	0	321	6	350	1.4674	0.0469	1.2671	2.9934	0.7166	13.3173		
CuCO3	61	2	128	339	6	307	1.5346	0.0501	1.0327	2.6884	0.255	10.3923	0.4845	
CuCO3	62	2	128	315	6	259	1.6551	0.0786	0.7973	3.0312	0.146	9.8852	0.5678	
CuCO3	63	2	128	364	6	430	1.4069	0.0688	1.07091	3.3998	0.2821	12.5933	0.5761	
CuCO3	64	2	128	342	6	310	1.2582	0.0865	1.1077	2.971	0.2016	10.2847	0.4036	
CuCO3	65	3	64	352	6	361	2.2009	0.051	1.2847	3.2906	0.7785	14.018	0.9786	
CuCO3	66	3	64	313	6	305	1.3726	0.0485	0.947	2.9637	0.4523	12.1044	0.9459	
CuCO3	67	3	64	346	6	369	0.9271	0.0487	1.2407	3.8061	0.8995	17.272	1.2716	
CuCO3	68	3	64	331	6	363	1.5333	0.0487	1.2407	3.0978	0.8355	13.2097	1.0405	
	69	4			6						0.7366		0.9598	_
CuCO3	70		32	329 327	-	364	1.5113	0.0578	1.0893	2.8763		14.47		
CuCO3		4			6	362	1.5213	0.0475	1.1675	2.9456	0.9803	13.8618	1.1389	
CuCO3	71	4	32	330	6	347	0.8275	0.0497	1.0867	3.135	0.4964	13.6816	0.6927	
CuCO3	72	4	32	342	6	374	1.5637	0.0542	1.2151	3.5063	0.9137	15.6645	1.2879	
CuCO3	73	5	16	335	6	372	1.5831	NA	1.2542	0.917	0.9812	14.8323	1.0689	
CuCO3	74	5	16	335	6	360	1.525	0.0458	1.2998	3.3714	0.7049	14.8755	0.9542	
CuCO3	75	5		319	6	351	1.3967	0.0496	1.1147	3.2236	0.6029	14.445	0.8447	
CuCO3	76	5	16	344	6	385	1.4849	0.0567	1.3063	3.13455	0.6915	15.0242	0.9536	_
CuCO3	77	6	8	320	6	350	1.4858	0.0468	1.214	3.1053	0.8092	13.8809	0.7785	
CuCO3	78	6	8	339	6	372	1.5469	0.0516	1.4147	2.7977	0.883	14.7633		
CuCO3	79	6	8	339	6	375	1.5061	0.0591	1.2927	3.5749	0.8327	15.0991	1.2186	
CuCO3	80	6	8	343	6	480	1.4469	0.0448	1.279	3.5775	0.7811	16.8317	0.977	
CuCO3	81	7	4	326	6	353	1.4554	0.0513	1.1751	3.6513	0.6818	13.9572	0.8631	
CuCO3	82	7	4	350	6	380	1.479	0.0434	1.3179	3.7768	0.7477	15,1913	0.9444	2
CuCO3	83	7	4	359	6	402	1.5213	0.0647	1.3176	2.9416	0.8102	17.576	1.2042	2 2
CuCO3	84	7	4	364	6	403	1.7883	0.0463	1.3064	3.3102	0.9161	15.9877	1.1483	3 2.
CuCO3	85	1	0	321	26	452	1.781	0.052	1.371	3.327	0.69	15.919	1.273)
CuCO3	86	1	0	345	26	456	1.737	0.058	1.398	3.431	1.042	15,158	1.103	3 3
CuCO3	87	1	0	347	26	475	2.072	0.027	1.386	3.736	0.809	18,789	1,191	1
CuCO3	88	1	0	337	26	443	1.65	0.049	1.271	3.524	0.567	15.21	0.878	3
CuCO3	89	2	128	345	6	284	1,4619	0.0712	0.8969	3,1924	0.1665	9.6909		
CuCO3	90	2	128	365	Ğ	311	1.4499	0.0661	0.9516	3.4607	0.1585	12.1347	0.7054	
CuCO3	91	2	128	319	6	274	1.1169	0.0621	0.9414	2.7137	0.1584	9.0967	0.341	
CuCO3	92	2	128	327	6	291	1.3328	0.0529	0.9213	2.8554	0.2813	10.8158	0.6404	
CuCO3	93	3	64	350	26				1.485	3.274	0.2813	18.278		
	93	3	64		26	467	1.131	0.048						
CuCO3		-		337		438	1.701	0.057	1.343	3.519	0.631	16.006	0.919	
CuCO3	95	3	64	335	26	429	1.493	0.05	1.304	3.143	0.632	14.066	1.083	
CuCO3	96	3	64	358	26	485	1.502	0.053	1.525	3.735	0.873	17.906	1.174	
CuCO3	97	4	32	327	26	434	1.595	0.052	1.368	3.32	0.561	14.2		
CuCO3	98	4	32	345	26	498	1.615	0.058	1.448	3.575	0.845	19.335	1.168	
CuCO3	99	4	32	338	26	449	1.495	0.046	1.363	3.288	0.848	15.307	1.146	
CuCO3	100	4	32	325	26	409	1.713	0.046	1.428	3.398	0.627	14.426	0.968	3
CuCO3	101	5	16	323	26	415	1.548	0.038	1.346	3.738	0.569	15.726	0.9227	,
CuCO3	102	5	16	336	26	446	1.767	0.039	1.324	3.663	0.764	16.66	1.056	5
CuCO3	103	5	16	350	26	468	1.711	0.057	1.43	3.818	0.663	16.078	1.164	ł
CuCO3	104	5	16	365	26	532	2.041	0.053	1.671	3.329	0.93	22.402	1.437	
CuCO3	105	6	8	323	26	449	1.62	0.058	1.384	3,491	0.668	16,146	1.151	

he following o	olumns contain a d	escription of the annotation that is used in the raw data files for all in-vovo work in by
_		a way that is is useful for analysis - in this case by PROAST software, or other datab
		n mathematical signs like %, +, -, /, (,). Instead of spaces to separate words, use _
.y descriptions	s should not contail	I mathematical signs like 76, +, -, 7, 1, (,). Instead of spaces to separate words, use _
1	subst	substance name
2	animal nr	animal number in the experiment
3	group_nr	group designation; 1 - 7
4	dose mg/kg	oral dose in mg/kg
5	body_wt day1	body weight at day 1 start of treatment in grams
6	autopsy day	day number of autopsy (6 or 26)
7	body wt	body weight at autopsy in grams
8	lung wt	lung weight in grams
9	adrenal wt	adrenal weight in grams
10	heart wt	heart weight in grams
11	testis wt	testis weight in grams
12	thymus wt	thymus weight in grams
13	liver wt	liver weight in grams
14	spleen wt	spleen weight in grams
15	kidney_wt	kindney weight in grams
16	mes LN wt	mesenterial Lymph nodes weight in grams
17	stomach wt	stomach weight in grams
18	brain wt	brain weight in grams
19.0	0 TP	Totap Proteine in gram per Liter
20	ALB	Albumin in gram per Liter
21	ALT	Alanine aminotransferase in IU per Liter
22	AST	Aspartaat aminotransferase in IU per Liter
23	ALP	Alkalic Phosphatase in IU per Liter
24	TBIL	Total Bilirubine in umol per Liter
25	YGTX	Gamma glutamyl traferase in U per Liter
26	LDP	Lactate dehydrogenase in IU per Liter
28	CHOL	Cholesterol in mmol per Liter
29	TG	Triglycerides in mmol per Liter
30	FFA	Free Fatty Acids in mmol per Liter
31	FE	Ferro in umol per Liter
32	ZINC	Zinc in ug per deciLiter
33	GLU	Glucose in mmol per Liter
34	CR S	Creatinine in umol per Liter
35	UREA	Urea in mmol per Liter
36	URIC	Uric Acid in umol per Liter
37	CA	Calcium in mg per deciLiter
38	CL	Chlorine in mmol per Liter
39	К	Potassium mmol per Liter
40	NA	Natrium in mmol per Liter
41	ROM	Reactive Oxygen Metabolites in U CARR ??
42	SHP	Plasmatic Thios Groups in umol per Liter
43	r ALT AST	ratio ALT/AST

Appendix 6: Eco-toxicology Test Method Description and Data Reporting Form

EUN – ECOTOXICOLOGY - TEST METHOD DESCRIPTION FORM

INFORMATION	ON TEST METHOD A	ND PROPOSER	/ PARTN	IER				
Name of test method	Eco-Toxicology of Nanoparticles to Benthic Organisms (<i>Lymnaea stagnalis</i>) <i>Lymnaea stagnali</i> s., Acute Lethal Test (Brix et al, 2011)							
Acronym of test method								
Proposer - Organisation	Organisation Name HWU	SUN WP ID WP4	SUN	Partner	D			
Postal address	Heriot-Watt University Currie, Edinburgh, Eh14 4as		·					
Name of contact person	Professor Teresa Fernandes PhD student Valentina Ricottone							
Tel. no. of contact person								
Fax no. of contact person								
e-mail of contact person	Vr77@hw.ac.uk							

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SUN WP1 STUDY DATABASE ADMIN USE ONLY

Received (Name/Date)	
Related data record files	
- (Excel Templates)	
Related characterisation file(s)	
DB Entry	
Check completion (Name/Date)	

1. Study Overview	
Test Material(s):	MWCNTs_1_NP_SYN WCCo_1_NP_SYN Pigment_1_NP_SYN (OrgPig Red254) CuO_1_NP_SYN CuSO4
OECD Test Name and Number:	No OECD standard test available
Duration of the test:	96 hours
Any deviations from the standard OECD protocol? (yes or no).	N/A
Species Used (latin name):	Lymnaea stagnalis
Strain of test organism:	<i>Lymnaea stagnalis</i> strain Renyls
Type of Media:	OECD 203

2. Study Protocol

Mortality was assessed through aqueous exposures by monitoring the mortality in a controlled light (16h d, 8h n) and temperature (20 °C) environment, following the protocol applied by Brix et al. (2011). Briefly, juvenile snails (7-9 day old) were placed in 35ml polypropylene containers with 30ml of test medium; three replicates of 15 snails were tested for each exposure concentration. Snails were left without food 24h prior the start the experiment. Exposure was performed over 96h, mortality recorded daily and snails were not fed during the experiment. Dose-response curves and EC10 and EC50 values and corresponding 95% confidence intervals were calculated using Sigmaplot.

3. Test Vessels Used

Test vessels are 35ml polypropylene containers with 30ml of test medium. Vessels were disposed after every experiment.

Duran bottle of 100ml where used for preparing NP stocks. Upon use with nanoparticles, the glassware was washed with Decon to remove major residuals and rinsed 3 x with H₂O and distilled H₂O.

4. Deviations from the study protocol

No deviations to the general study protocol.

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SUN Ecotoxicology Template: Test Method Description Form



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5. Source of Test Organism and Routine Husbandry

Lymnaea stagnalis used for these experiments are from the strain Renyls. They are cultured in OECD 203 media, pH in the range 7-8 and water hardness of 78 mg CaCo3/L, ammonia low than 2 mg/L. Snails are cultured at room temperature in a natural light regime. Snails are fed at libitum with only lettuce to avoid increasing of ammonia concentration. They are kept in a 10 L plastic tank at the density of 300ml /snail. Twice a week one third of the water is changed and all the clutches removed and placed in another tank in order to have cohorts of snails with similar age and (roughly) similar size. At 20°C and renew the water twice per week, a 3 cm adult produces 2 clutches of approx 80 eggs per week. The number of embryos per clutch increase linearly with the adult's size. Embryos hatch after 15 to 30 days at 20°C, and they need 3 months to start reach sexual maturity.

6. Source and Chemical Composition of the Test Media

OECD 203 for Lymnaea stagnalis

- Calcium chloride solution
 Dissolve 11.76 g CaCl₂.2H₂0 in deionised water, make up to 1 litre with deionised water
- (b) Magnesium sulphate solution Dissolve 4.93 g MgS0_e.7H₂0 in deionised water, make up to 1 litre with deionised water
- (c) Sodium bicarbonate solution Dissolve 2.59 g NaHC0, in deionised water, make up to 1 litre with deionised water
- (d) Potassium chloride solution Dissolve 0.23 g KCl in deionised water, make up to 1 litre with deionised water

All chemicals must be of analytical grade.

The conductivity of the distilled or deionised water should not exceed 10 µScm⁻¹.

25 ml each of solutions (a) to (d) are mixed and the total volume made up to 1 litre with deionised water. The sum of the calcium and magnesium ions in this solutions is 2.5 mmol/l. The proportion Ca:Mg ions is 4:1 and Na:K ions 10:1. The acid capacity K_{S43} of this solution is 0.8 mmol/l.

Aerate the dilution water until oxygen saturation is achieved, then store it for about two days without further aeration before use.

2. Evidence That The Test Conditions Were Generally Met

In all experiments, the pH values along with the oxygen content were mostly stable. During the tests, not more than 10 percent of the control *snails* died.



Parameter	Diamont 4	WCCo_1_	CuO_1_N	CuSO₄*5H	MMONTA
Parameter	Pigment_1_ NP_SYN (OrgPig Red254)	NP_SYN	P_SYN	20 20	MWCNTs_ _NP_SYN
Mass concentration of the stock dispersion.	0.1mg/ml	0.1mg/ml	0.08mg/ml Cu	0.0025mg/ ml Cu	1mg/ml
What the material is dispersed in (e.g., ultrapure water, 10% alcohol, soil, etc.) including pre- wetting steps and use of stabilizers.	0.01g of NP in 100ml of MilliQ water	0.01g of NP in 100ml of 0.01% (wt/vol) sodium polyphosph ate	0.01g of NP in 100ml of MilliQ water	0.001g of chemical in 100ml of MilliQ water	0.01g of NP in 100ml of 0.2 % SRHA 1g L ⁻¹
For secondary stock made from another solution, indicate how the original was diluted.					
Sonication (including type of sionicator, energy and time) or stirring (stirring speed and time) to disperse the stock.	NPs in a 100 mL duran bottle were sonicated for 8+8 minutes with bath sonicator following Jacobsen 2010 protocol	NPs in a 100 mL duran bottle were sonicated for 8+8 minutes with bath sonicator following Jacobsen 2010 protocol	NPs in a 100 mL duran bottle were sonicated for 8+8 minutes with bath sonicator following Jacobsen 2010 protocol	Chemical in a 100 mL duran bottle was stirred for 5 minutes	NPs in a 100 mL duran bottle were sonicated fo 16 minutes four times with bath sonicator following Jacobsen 2010 protoc
Storage conditions and time (if relevant).	NPs prepared on the same day of the experiment	NPs prepared on the same day of the experiment	NPs prepared on the same day of the experiment	Solution is prepared on the same day of the experiment	NPs prepared on the same da of the experiment
Media used to make any working dilutions of the stock. Primary particle size (indicate diameter)					



SUN Ecotoxicology Template: Test Method Description Form



size distribution by DLS.			
Any measured impurities that are relevant.			

9. Dosing of the Test Vessels

Depending the concentration of NP wanted in the test vessel, aliquote from the stock dispersion where pipetted in the test vessel containing 30 ml of media. The media was then topped up to reach the volume of 38ml.

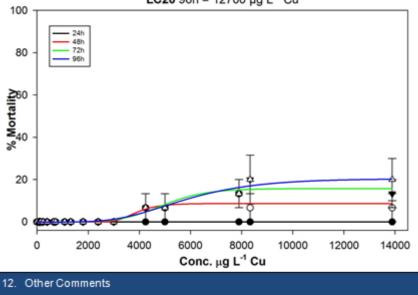
10. Nanomaterial Concentration During the Test

No measurements were performed.

11. RESULTS

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Organisms exposed to WC-Co NPs and MWCNTs in the range of concentrations investigated (0-21000 μ g L-1) showed no mortality (data not reported). Exposure to Org. Pig. Red254 indicated lethal concentration values (LC20) mortality to 20% of the population at 96h of 12700 μ g L⁻¹ at 96h (Fig. 16) of Org. Pig. Red 254 to *L. stagnalis.*



Acute exposure Org. Pig. Red254 juveniles Lymnaea stagnalis LC20 96h = 12700 μg L⁻¹ Cu

TEST CONDITIONS	Please comp	lete the de	etails bel	ow as far a	as possibl	le fe	
Ecotoxicology	Whilst aiming to You can add ad In the notes are	ditional item	ns below v	vhere nece	ssary for f	urth	
TEST and END POINT - GENERAL INFO							
MARINA Work Package: Partner ID:	10 AU						
Test facility - Lab name etc: Work conducted by:	AU Janeck J.Scott-Ford	dsmand	email	address:	jsf@bios.au	u.dk	
Test / Assay End-Point short description: (Enter full description in the covering TMDF - assay description for	Multispecies test orm)						
End-Point Outcome metric (ie % viability, %cell death etc): (indicate how EP is derived)	Total Population Total Population Total Population						
SOP - Protocol Name - ID (see project protocol ID list): (or add path/link to protocol on server)	Based on Scott-For	dsmand et al	2008, Envir	onment Interr	national		
Test start date (dd/mm/yyyy): Test end date (dd/mm/yyyy):	22/10/2013 19/11/2013						
TEST SUBSTANCE							
Substance name: CAS No:	CuO_1_NP_PEI	CuO_1_NF	P_PVP; C	uO_1_NP_	CITRATE;	Сι	
Standard Nanomaterial Code & Name: (See Materials list; or other standard list eg JRC) Highest concentration, inc units:	NMXXX 1280	ma Aa/ka				-	
DISPERSION	1200	ing Ag/kg					
Specify the standard dispersion protocol used: (or otherwise specify the dispersion technique used)	none						
Dispersion agent:	none						
Aids used to disperse - Y / N:	Sonication:	none	Vortexing	none	Stiring:	no	
Treatment concentration series (C) (mg/Kg):	C1	C2	C3	C4	C	5	
Icst conditions Raw data Test results	series (C) (mg/Kg): C1 C2 C3 C4 C5						

Appendix 7: Eco-toxicology data collection template

A	В	C	D	E	F	G	Н		J	K
RAW DATA		Insert uor	ir results ap	propriate l	to your exp	erimental	eaime			
			ates that a					nsert anu d	iait)	
	Total P	opulatio	n							
			Species	Species	Species	Species	Species	Benl7		
	Control		1648	461	51	20	11			
	Citrate		1031	404	86	15	6			
	Ascorb		1621	529	51	8	š			
	PEI	743	1609	528	61	22	10			
	PYP	279	1368	486	71	19	10			
	0	2.10								
	0									
	Ő									
	0									
	Total P	opulatio	n							
			Species	Snecies	Species	Snecies	Snecies	Benl7		
	Control		1423	413	19	7	107	. iepii		
										-
	Citrate		943	315	11	2	100			_
	Ascorb	77	888	300	7	6	81			
	PEI	820	1067	365	9	3	112			
	PVP	212	1078	426	15	3	107			
	0									
	0									
	0									
	0									
	Total P	opulatio	n							
			Species	Species	Species	Species	Species	Repl7		
	Control		1538	190	1	2	48			
	Citrate		891	70	0	0	117			
	Ascorb		1076	110	0	0	64			
	PEI	580	1152	119	0	0	51			
	PVP	142	1264	84	0	0	103			
	0				-	· · · · · ·				
	0									
	0									
	0									
	0									
		Species	Species	Species	Species	Species	Species	Repl7		
	Citrate									
	Ascorb	ate								
	PEI									
	PVP									
	*#REF!									
	0									
	0									
	0									

RESULTS						
	Total Population					
	28 days	CuO_1_NP_PELC	Averag	ge raw data	×	
		Citrate		473.167		100.000
		Ascorbate		293.833		62.099
		PEI		406.667		85.946
		PVP		495.500		104.720
		#REF!		372.167		78.654
		0		#DIV/0!		#DIV/0!
		0		#DIV/0!		#DIV/0!
		0		#DIV/0!	•	#DIV/0!
		0		#DIV/0!	•	#DIV/0!
	Total Population					
	56 days	CuO_1_NP_PELC	Avera	ge raw data	×	
		Citrate		477.667		100.000
		Ascorbate		244.500		51.186
		PEI		226.500		47.418
		PVP		396.000		82.903
		#REF!		306.833		64.236
		0		#DIV/0!	•	#DIV/0!
		0		#DIV/0!	•	#DIV/0!
		0		#DIV/0!		#DIV/0!
		0		#DIV/0!		#DIV/0!
		•		in Existence		in Diffici.
	Total Population					
	84 days	CuO_1_NP_PELC	A uora	e teb wer or	z	
	04 days	Citrate	CALCE OF	415.167	~	100.000
		Ascorbate		213.167		51.345
		PEI		240.833		58.009
		PVP		317.000		76.355
		#REF!		265.500		63.950
		0		#DIV/0!	-	#DIV/0!
		0	_	#DIV/0!		#DIV/0!
		0		#DIV/0!	_	#DIV/0!
		0	·	#DIV/0!	r	#DIV/0!
	0		A			
	U U	CuO_1_NP_PELC	Averag		7	#01/2/01
		Citrate		#DIV/0!		#DIV/0!
		Ascorbate		#DIV/0!	-	#DIV/0!
		PEI		#DIV/0!	_	#DIV/0!
		PVP		#DIV/0!	<u> </u>	#DIV/0!
		#REF!		#DIV/0!	<u> </u>	#DIV/0!
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