

**HORIZON
2020**

Development and Implementation of a Sustainable Modelling Platform for NanoInformatics.

Resultados

Información del proyecto

NanoInformaTIX

Identificador del acuerdo de subvención:
814426

[Sitio web del proyecto](#) 

DOI

[10.3030/814426](https://doi.org/10.3030/814426) 

Proyecto cerrado

Fecha de la firma de la CE

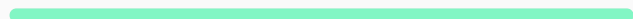
12 Diciembre 2018

Fecha de inicio

1 Enero 2019

Fecha de finalización

28 Febrero 2023



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INDUSTRIAL LEADERSHIP - Leadership in enabling and industrial technologies - Advanced materials

Coste total

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Aportación de la UE

€ 6 783 556,25

Coordinado por

AGENCIA ESTATAL CONSEJO
SUPERIOR DE
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 España

Este proyecto figura en...

Investigación sobre materiales avanzados para aplicaciones industriales y la sociedad

CORDIS proporciona enlaces a los documentos públicos y las publicaciones de los proyectos de los programas marco HORIZONTE.

Los enlaces a los documentos y las publicaciones de los proyectos del Séptimo Programa Marco, así como los enlaces a algunos tipos de resultados específicos, como conjuntos de datos y «software», se obtienen dinámicamente de [OpenAIRE](#) .

Resultado final

Documentos, informes (15)

[Strategy to calculate in vivo exposure dose based on the modelling strategies developed in NanoInformaTIX](#) 

TMK will develop a strategy based on the collected in vitro and in vivo data to predict exposure doses

[Report on application and integration of data analysis method for data curation and data exploration](#) 

Report on the methods applied and/or developed and their impact on the NanoInformaTIX database

[Overview of available data, modelling methods and modelling tools requirements](#) 

This report will provide overview of data of interest to NanoInformaTIX framework, modelling methods and tools envisaged for integration, and their specific requirements (data quality, e.g. input and output formats)

[Workflows integrating ontology into data curation, data validation and input/output of modelling tools will be defined](#) 

Workflows for ontology supported data curation and validation including data quality and completeness criteria will be described

[Human exposure models](#)

This deliverable will present the final human NanoInformaTIX models that describe indoor exposure modeling of ENM

[Test design recommendations for an ENM systems toxicology approach using non animal alternative test methods](#)

Based on systems biology guidance on best practices and test design will be given focussing on the specificities of testing ENM UAVR will draft and all WP5 partners will contribute

[Human PBPK Modeling](#)

This deliverable will report the final development of the human PBPK models developed within NanoInformaTIX

[Developing an integrative analysis pipeline for multi-omics data for defining MIEs and Key Events of ENM](#)

UFZ will report on the development of an integrative analysis pipeline for multiomics data

[Environmental exposure models](#)

This deliverable will present the final environmental NanoInformaTIX models that describe release and environmental fate modeling of ENM providing the environmental dose

[Report on ontology usage and requirements Workflow for ontological development and maintenance](#)

-Existing ontologies will be analysed and list of new ontology entries will be proposed to maintainers of eNanoMapper and EMMO ontology. A workflow enabling continuous update and maintenance of the ontology will be described, in collaboration with existing ontology development communities.

[Open source libraries for interaction with NanoInformaTIX database](#)

This deliverable will describe the open source libraries implemented by T24 enabling interoperable communication with NanoInformaTIX database Application to answering specific scientific questions and integration with modelling tools will be described

[1 NanoInformaTIX database release](#)

This report will describe the technical implementation and content of NanoInformaTIX database release Iterative development and releases at M12 M24 and M36 are planned based on requirement identified by T22 partners feedback and developments in T23T25

[Mode of action grouping of ENM based on advanced material descriptors](#)

NTUA will provide a report on the mode of action grouping of ENM based on advanced material descriptors

[Plan for stakeholder events and trainings](#)

We will have two stakeholder events (together with WP7) to gather feedback on the development of the SNF Platform. We will also run annual training schools, if possible together with other EC funded initiatives, to transfer knowledge to the next generation of researchers, and a final event to disseminate the projects' results to stakeholders

[Dose-response modelling](#)

Report summarizing the doseresponse models developed within task 51

Open Research Data Pilot (1)



[NanoInformaTIX Data Management Plan](#)

This report will provide the first version of DMP describing the NanoInfomaTIX approach to data collection, management and curation.

Conjuntos de datos, microdatos, etc. (1)



[Database on ENM biodistribution](#)

In this database the available data on ENM biodistribution (environmental, human) will be collected.

Demostradores, pilotos, prototipos (1)



[Safe-by-Design approach and corresponding platform](#)

DEMOKRITOS will provide a description of the developed approach for “safe-by-design”, which will take into account the feedbacks collected also by WP4, WP5 and WP6. NCSR will be responsible for developing a software tool to guide the reverse engineering towards safe-by-design materials.

Sitios web, solicitudes de patentes, vídeos, etc. (1)



[Communication Basics](#)

Otro (2)

[Hybrid material models for computing physicochemical descriptors of ENM](#) 

This deliverable is an update of the D31 and hence the same format applies. In particular, the same consistency requirements with regards to EMMC recommendations will be adopted. This deliverable will include a set of datasheets about material models which may also include experimental results and hence are defined as hybrid. This corresponds to the critical decision: main path or alternative which will be taken at M24 by D31. These datasheets will report i) the hybrid material modelling workflows and ii) the corresponding estimated values about advanced descriptors as specified in WP45. Each estimated descriptor will be reported with the corresponding uncertainty for validation purposes in WP6.

[Pure material models for computing physicochemical descriptors of ENM](#) 

POLITO will prepare a set of datasheets about material models for computing physicochemical descriptors of ENM in a format agreed with the leading partners involved in material modelling in T3a beforehand. The datasheets will be in line with the requirements of the MOdelling DAta MODA approach (<https://www.ceneuNewsWorkshops/Pages/WS2017012.aspx>) and with the European Materials Modelling Ontology (EMMO) for semantic interoperability (<http://semmc.info>). These datasheets will report i) the material modelling workflows and ii) the corresponding computed values about the preliminary list of advanced descriptors agreed in D33 at M12. Each computed descriptor will be reported with the corresponding uncertainty for validation in WP6.

Publicaciones

Otro (2)

[International Network Initiative on Safe and Sustainable Nanotechnologies \(INISS-nano\)](#) 

Autores: Falk, Andreas

Publicado en: Edición 12, 2021

Editor: BioNanoNet

DOI: 10.5281/zenodo.5004929

[Editorial for the Special Issue From Nanoinformatics to Nanomaterials Risk Assessment and Governance.](#) 

Autores: Iseult Lynch; Antreas Afantitis; Dario Greco; Maria Dusinska; Miguel A. Bañares; Georgia Melagraki

Publicado en: Nanomaterials, Edición 11/2021, 2021, Página(s) p 121, ISSN 2079-4991

Editor: MDPI

DOI: 10.3390/nano11010121

Artículos arbitrados (33)

[Transcriptomics in Toxicogenomics, Part I: Experimental Design, Technologies, Publicly Available Data, Regulatory Aspects](#) 

Autores: Pia Anneli Sofia Kinaret, Angela Serra, Antonio Federico, Pekka Kohonen, Penny Nymark, Irene Liampa, My Kieu Ha , Jang-Sik Choi, Karolina Jagiello, Natasha Sanabri, Georgia Melagraki, Luca Cattelani, Michele Fratello, Haralambos Sarimveis6, Antreas Afantitis , Tae-Hyun Yoon, Mary Gulumian, Roland Grafström, Tomasz Puzyn, Dario Greco

Publicado en: Nanomaterials, Edición 10(4), 750, 2020, ISSN 2079-4991

Editor: MDPI

DOI: 10.3390/nano10040750

[Size-Specific, Dynamic, Probabilistic Material Flow Analysis of Titanium Dioxide Releases into the Environment.](#) 

Autores: Yuanfang Zheng; Bernd Nowack

Publicado en: Environmental Science & Technology, Edición 55, 4, 2021, Página(s) 2392–2402, ISSN 1520-5851

Editor: American Chemical Society

DOI: 10.1021/acs.est.0c07446

[Annelid genomes: Enchytraeus crypticus, a soil model for innate \(and primed\) immune system](#) 

Autores: Mónica J.B. Amorim, Yannick Gansemans, Susana I.L. Gomes, Filip Van Nieuwerburgh and Janeck J. Scott-Fordsmand

Publicado en: Lab Animal, Edición 50, 285–294 (2021), 2021, ISSN 0093-7355

Editor: Nature Publishing Group

DOI: 10.1038/s41684-021-00831-x

[Effects of natural organic matter on the joint toxicity and accumulation of Cu nanoparticles and ZnO nanoparticles in Daphnia magna](#) 

Autores: Qi Yu, Zhuang Wang, Guiyin Wang, Willie J. G. M. Peijnenburg, Martina G. Vijver

Publicado en: Environmental Pollution, Edición Volume 292, Part B, 1 January

2022, 118413, 2022, ISSN 0269-7491

Editor: Pergamon Press Ltd.

DOI: 10.1016/j.envpol.2021.118413

[""Systems toxicology to advance human and environmental hazard assessment: A roadmap for advanced materials""](#) 

Autores: M.J.B. Amorim, W. Peijnenburg, D. Greco, L.A. Saarimäki, V.I. Dumit f, A. Bahl, A. Haase, L. Tran, J. Hackermüller, S. Canzler, J.J. Scott-Fordsmand

Publicado en: Nano Today, Edición 48 (February 2023), 2023, ISSN 1748-0132

Editor: Elsevier BV

DOI: 10.1016/j.nantod.2022.101735

[Probing Nano-QSAR to Assess the Interactions between Carbon Nanoparticles and a SARS-CoV-2 RNA Fragment](#) 

Autores: Fan Zhang, Zhuang Wang, Martina G. Vijver, Willie J.G.M. Peijnenburg

Publicado en: Ecotoxicology and Environmental Safety, Edición Volume 219, August 2021, 112357, 2021, ISSN 1090-2414

Editor: Orlando, Fla. Academic Press

DOI: 10.1016/j.ecoenv.2021.112357

[Machine learning and materials modelling interpretation of in vivo toxicological response to TiO2 nanoparticles library \(UV and non-UV exposure\)](#) 

Autores: Susana I. L. Gomes; Mónica J. B. Amorim; Suman Pokhrel; Lutz Mädler; Matteo Fasano; Eliodoro Chiavazzo; Pietro Asinari; Jaak Jänes; Kaido Tamm; Jaanus Burk; Janeck J. Scott-Fordsmand

Publicado en: Nanoscale, Edición 35/2021, 2021, ISSN 2040-3372

Editor: Royal Society of Chemistry

DOI: 10.1039/d1nr03231c

[BMDx: a graphical Shiny application to perform Benchmark Dose analysis for transcriptomics data](#) 

Autores: Angela Serra, Laura Aliisa Saarimäki, Michele Fratello, Veer Singh Marwah, Dario Greco

Publicado en: Bioinformatics, Edición Volume 36, Edición 9, 2020, ISSN 1367-4811

Editor: Oxford University Press

DOI: 10.1093/bioinformatics/btaa030

[Pulmonary toxicity of silver vapours, nanoparticles and fine dusts: A review](#) 

Autores: Niels Hadrup, Anoop K. Sharma, Katrin Loeschner, Nicklas R. Jacobsen

Publicado en: Regulatory Toxicology and Pharmacology, Edición 115, 2020, Página(s) 104690, ISSN 0273-2300

Editor: Academic Press

DOI: 10.1016/j.yrtph.2020.104690

[Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields](#) 

Autores: Brajesh Narayan; Colm Herbert; Brian J. Rodriguez; Bernard R. Brooks; Nicolae-Viorel Buchete

Publicado en: The Journal of Physical Chemistry. B, Edición 125, 20, 2021, Página(s) 5233–5242, ISSN 1089-5639

Editor: American Chemical Society

DOI: 10.1021/acs.jpcc.1c01939

[Trophic transfer of Cu nanoparticles in simulated aquatic food chains](#) 

Autores: Qi Yu, Zhuang Wang, Willie J. G. M. Peijnenburg, Martina G. Vijver

Publicado en: Ecotoxicology and Environmental Safety, Edición Volume 242, 1 September 2022, 113920, 2022, ISSN 1090-2414

Editor: Orlando, Fla. Academic Press

DOI: 10.1016/j.ecoenv.2022.113920

[A systematic quality evaluation and review of nanomaterial genotoxicity studies – a regulatory perspective](#) 

Autores: Siivola KM, Burgum MJ, Suárez-Merino B, Clift M, Doak S and Catalán J

Publicado en: Particle and Fibre Toxicology, Edición 2022; 19: 59, 2022, ISSN 1743-8977

Editor: BioMed Central

DOI: 10.1186/s12989-022-00499-2

[Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning](#) 

Autores: Brajesh Narayan; Nicolae-Viorel Buchete; Ron Elber

Publicado en: Journal of Physical Chemistry B, 2021, ISSN 1089-5639

Editor: American Chemical Society

DOI: 10.1021/acs.jpcc.1c00264

[Core, Coating, or Corona? The Importance of Considering Protein Coronas in nano-QSPR Modeling of Zeta Potential.](#) 

Autores: Selvaraj Sengottayan, Alicja Mikolajczyk, Karolina Jagiełło, Marta Swirow, and Tomasz Puzyn

Publicado en: ACS Nano, Edición Vol 17, Edición 3, 2023, ISSN 1936-0851

Editor: American Chemical Society

DOI: 10.1021/acsnano.2c06977

[Assembling Biocompatible Polymers on Gold Nanoparticles: Towards a Rational Design of Particle Shape by Molecular Dynamics](#) 

Autores: Roberta Cappabianca, Paolo De Angelis, Annalisa Cardellini, Eliodoro Chiavazzo and Pietro Asinari

Publicado en: ACS Omega, Edición 2022, 7, 46, 2022, ISSN 2470-1343

Editor: ACS Publications

DOI: 10.1021/acsomega.2c05218

[PROTEOMAS: a workflow enabling harmonized proteomic meta-analysis and proteomic signature mapping](#)

Autores: Aileen Bahl, Celine Ibrahim, Kristina Plate, Andrea Haase, Jörn Dengjel, Penny Nymark & Verónica I. Dumit

Publicado en: Journal of Cheminformatics, Edición 15, Article number:34, 2023, ISSN 1758-2946

Editor: Chemistry Central

DOI: 10.1186/s13321-023-00710-2

[Development of a quasi-QSAR model for prediction of the immobilization response of Daphnia magna exposed to metal-based nanomaterials](#)

Autores: Warisa Bunmahotama, Martina G. Vijver, Willie Peijnenburg

Publicado en: Environmental Toxicology and Chemistry, Edición 2022 Jun; 41(6): 1439–1450., 2022, ISSN 1552-8618

Editor: Society of Environmental Toxicology and Chemistry

DOI: 10.1002/etc.5322

[Multi-Scale Modelling of Aggregation of TiO₂ Nanoparticle Suspensions in Water](#)

Autores: G.Mancardi(POLITO), M.Alberghini(POLITO), N.Aguilera-Porta(Sorbonne), M.Calatayud(Sorbonne), P.Asinari(POLITO&INRIM) and E.Chiavazzo(POLITO)

Publicado en: nanomaterials, Edición 2(2), 217, 2022, ISSN 2079-4991

Editor: MDPI

DOI: 10.3390/nano12020217

[multiGSEA: a GSEA-based pathway enrichment analysis for multi-omics data.](#)

Autores: Sebastian Canzler; Jörg Hackermüller

Publicado en: BMC Bioinformatics, Edición 21/2020, 2020, ISSN 1471-2105

Editor: BioMed Central

DOI: 10.1186/s12859-020-03910-x

[Meta-analysis of Bioaccumulation Data for Nondissolvable Engineered Nanomaterials in Freshwater Aquatic Organisms](#)

Autores: Yuanfang Zheng; Bernd Nowack

Publicado en: Environmental Toxicology and Chemistry, Edición Volume 41, Edición 5, 2022, Página(s) Pages 1202-1214, ISSN 1552-8618

Editor: SETAC

DOI: 10.1002/etc.5312

[Multiomics assessment in Enchytraeus crypticus exposed to Ag nanomaterials \(Ag NM300K\) and ions \(AgNO3\) – Metabolomics, proteomics \(& transcriptomics\)](#) 

Autores: Vera L. Maria; David Licha; Janeck J. Scott-Fordsmand; Christian G. Huber; Mónica J.B. Amorim

Publicado en: Environmental Pollution, Edición 286, 2021, ISSN 1873-6424

Editor: Elsevier

DOI: 10.1016/j.envpol.2021.117571

[Alternative test methods for \(nano\)materials hazards assessment: challenges and recommendations for regulatory preparedness](#) 

Autores: Susana I.L. Gomes, Janeck J. Scott-Fordsmand and Monica J.B. Amorim

Publicado en: Nano Today, Edición Volume 40, October 2021, 101242, 2021, ISSN 1748-0132

Editor: Elsevier BV

DOI: 10.1016/j.nantod.2021.101242

[Toxicokinetics and toxicodynamics of Ag nanomaterials \(NM300K\) in the soil environment – impact on Enchytraeus crypticus \(Oligochaeta\)](#) 

Autores: Fátima C.F. Santosa, Rudo A. Verweijb, Cornelis A.M. van Gestelb and Mónica J.B. Amorima

Publicado en: Ecotoxicology and Environmental Safety, Edición Volume 252, 1 March 2023, 114599, 2023, ISSN 0147-6513

Editor: Academic Press

DOI: 10.1016/j.ecoenv.2023.114599

[Graphene nanoplatelets and reduced graphene oxide elevate the microalgal cytotoxicity of nano-zirconium oxide.](#) 

Autores: Zhuang Wang; Fan Zhang; Martina G. Vijver; Willie J.G.M. Peijnenburg

Publicado en: Chemosphere, Edición 276, 2021, ISSN 1879-1298

Editor: Elsevier

DOI: 10.1016/j.chemosphere.2021.130015

[Epigenetic effects of \(nano\)materials in environmental species – Cu case study in Enchytraeus crypticus](#) 

Autores: Rita C. Bicho, Dick Roelofs, Janine Mariën, Janeck J. Scott-Fordsmand, Mónica J.B. Amorim

Publicado en: Environment International, Edición 136, 2020, Página(s) 105447, ISSN 0160-4120

Editor: Pergamon Press Ltd.

DOI: 10.1016/j.envint.2019.105447

[Aquatic Mesocosm Strategies for the Environmental Fate and Risk Assessment of Engineered Nanomaterials.](#) 

Autores: Andrea Carboni; Danielle L. Slomberg; Mohammad Nassar; Catherine Santaella; Armand Masion; Jérôme Rose; Mélanie Auffan

Publicado en: <https://hal-cnrs.archives-ouvertes.fr/hal-03468409>, Edición 2, 2021, ISSN 0013-936X

Editor: American Chemical Society

DOI: 10.1021/acs.est.1c02221

[Comparison of Biokinetic Models for Non-dissolvable Engineered Nanomaterials in Freshwater Aquatic Organisms](#) 

Autores: Yuanfang Zheng, Bernd Nowack

Publicado en: Environmental Science: Nano, Edición 2023,10, 1065-1076, 2023, ISSN 2051-8161

Editor: Royal Society of Chemistry

DOI: 10.1039/d2en01039a

[Multivariate analysis of the exposure and hazard of ceria nanomaterials in indoor aquatic mesocosms](#) 

Autores: Mohammad Nassar; Mélanie Auffan; Mélanie Auffan; Catherine Santaella; Armand Masion; Jérôme Rose; Jérôme Rose

Publicado en: Environmental Science Nano, Edición 6/2020, 2020, ISSN 2051-8161

Editor: Royal Society of Chemistry

DOI: 10.1039/c9en01439j

[The role of size and nature in nanoparticle binding to a model lung membrane: an atomistic study](#) 

Autores: Ankush Singhal; Geert Jan Agur Sevink

Publicado en: Nanoscale Advances, Edición 23/2021, 2021, ISSN 2516-0230

Editor: Royal Society of Chemistry

DOI: 10.1039/d1na00578b

[Your Spreadsheets Can Be FAIR: A Tool and FAIRification Workflow for the eNanoMapper Database](#) 

Autores: Nikolay Kochev, Nina Jeliaskova, Vesselina Paskaleva, Gergana Tancheva, Luchesar Iliev, Peter Ritchie, Vedrin Jeliaskov

Publicado en: Nanomaterials, Edición 10/10, 2020, Página(s) 1908, ISSN 2079-4991

Editor: MDPI

DOI: 10.3390/nano10101908

[Predicting electrophoretic mobility of TiO₂, ZnO and CeO₂ nanoparticles in natural waters: The importance of environment descriptors in nanoinformatics models](#) 

Autores: Marta Swirog, Alicja Mikołajczyk, Karolina Jagiello, Jaak Jänes, Kaido Tamm, Tomasz Puzyn

Publicado en: Science of the Total Environment, Edición Volume 840, 20

September 2022, 156572, 2022, ISSN 1879-1026

Editor: Elsevier

DOI: 10.1016/j.scitotenv.2022.156572

[Multigenerational Exposure to WCCo Nanomaterials—Epigenetics in the Soil Invertebrate *Enchytraeus crypticus*](#) 

Autores: Rita C. Bicho, Janeck J. Scott-Fordsmand, Mónica J.B. Amorim

Publicado en: Nanomaterials, Edición 10/5, 2020, Página(s) 836, ISSN 2079-4991

Editor: MDPI

DOI: 10.3390/nano10050836

[How Does the Study MD of pH-Dependent Exposure of Nanoparticles Affect Cellular Uptake of Anticancer Drugs?](#) 

Autores: Selvaraj Sengottayan, Alicja Mikolajczyk, Tomasz Puzyn

Publicado en: International Journal of Molecular Sciences, Edición Vol 24, Edición 4, 2023, ISSN 1422-0067

Editor: Multidisciplinary Digital Publishing Institute (MDPI)

DOI: 10.3390/ijms24043479

Actas de congresos (1)

""Fostering EU-US Cooperation in Nanosafety""

Autores: Miguel Bañares

Publicado en: 2019

Editor: Harvard University

Conjuntos de datos

Conjuntos de datos vía OpenAIRE (2)



[ss-PDMFA: size-specific, probabilistic, dynamic material flow analysis](#) 

Autores: Zheng Yuanfang; Nowack Bernd

Publicado en: Zenodo

[Classification of GTP-dependent K-Ras4B active and inactive conformational states](#) 

Autores: Narayan, Brajesh; Kiel, Christina; Buchete, Nicolae-Viorel
Publicado en: Zenodo

Otros productos de investigación

Otros productos de investigación a través de OpenAire (1)



[Data & code repository for the article "An ancestral molecular response to nanomaterial particulates"](#)



Autores: Giudice, Giusy Del; Greco, Dario

Publicado en: Zenodo

Última actualización: 11 Diciembre 2023

Permalink: <https://cordis.europa.eu/project/id/814426/results/es>

European Union, 2025