Development and Implementation of a Sustainable Modelling Platform for NanoInformatics.

Wyniki

Informacje na temat projektu

NanoInformaTIX

Identyfikator umowy o grant: 814426

Strona internetowa projektu

DOI
10.3030/814426

Projekt został zamknięty

Data podpisania przez KE
12 Grudnia 2018

Data rozpoczęcia
1 Stycznia 2019

Data zakończenia
28 Lutego 2023

Finansowanie w ramach
INDUSTRIAL LEADERSHIP - Leadership in enabling and industrial technologies - Advanced materials

Koszt całkowity
€ 7 751 271,25

Wkład UE
€ 6 783 556,25

Koordynowany przez
AGENCIA ESTATAL CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS
Hiszpania

Ten projekt został przedstawiony w...

5 Czerwca 2023

CORDIS oferuje możliwość skorzystania z odnośników do publicznie dostępnych publikacji i rezultatów projektów realizowanych w ramach programów ramowych HORYZONT.

Odnośniki do rezultatów i publikacji związanych z poszczególnymi projektami 7PR, a także odnośniki do niektórych konkretnych kategorii wyników, takich jak zbiory danych i oprogramowanie, są dynamicznie pobierane z systemu OpenAIRE.

Rezultaty

Dokumenty, raporty (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 andor 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

eport 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.

Zestawy danych, mikrodane itp. (1)

Database on ENM biodistribution

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

Demonstratory, piloty, prototypy (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.

Witryny, zgłoszenia patentowe, filmy wideo itp. (1)

Communication Basics

Logo, website, brochure, presentation template

Inne (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 httpsemmcinfo 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 httpswwwceneuNewsWorkshopsPagesWS2017012aspx and with the European Materials Modelling Ontology EMMO for semantic interoperability httpsemmcinfo These datasheets will report i the material modelling workflows and ii the corresponding computed values about the preliminary list of advanced descriptors WP45 agreed in D33 at M12 Each computed descriptor will be reported with the corresponding uncertainty for validation WP6

Publikacje

Inne (2)

International Network Initiative on Safe and Sustainable Nanotechnologies (INISS-nano)

Autorzy: Falk, Andreas
Opublikowane w: Numer 12, 2021
Wydawca: BioNanoNet
DOI: 10.5281/zenodo.5004929

Editorial for the Special Issue From Nanoinformatics to Nanomaterials Risk Assessment and Governance.

Autorzy: Iseult Lynch; Antreas Afantitis; Dario Greco; Maria Dusinska; Miguel A. Bañares; Georgia Melagraki
Opublikowane w: Nanomaterials, Numer 11/2021, 2021, Strona(/y) p 121, ISSN 2079-4991
Wydawca: MDPI
DOI: 10.3390/nano11010121

Artykuły recenzowane (33)

Transcriptomics in Toxicogenomics, Part I: Experimental Design, Technologies, Publicly Available Data, Regulatory Aspects

Autorzy: 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
Opublikowane w: Nanomaterials, Numer 10(4), 750, 2020, ISSN 2079-4991
Wydawca: MDPI
DOI: 10.3390/nano10040750

Size-Specific, Dynamic, Probabilistic Material Flow Analysis of Titanium Dioxide Releases into the Environment.

Autorzy: Yuanfang Zheng; Bernd Nowack
Opublikowane w: Environmental Science & Technology, Numer 55, 4, 2021, Strona(/y) 2392–2402, ISSN 1520-5851
Wydawca: American Chemical Society
DOI: 10.1021/acs.est.0c07446

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

Autorzy: Mónica J.B. Amorim, Yannick Gansemans, Susana I.L. Gomes, Filip Van Nieuwerburgh and Janeck J. Scott-Fordsmand
Opublikowane w: Lab Animal, Numer 50, 285–294 (2021), 2021, ISSN 0093-7355
Wydawca: 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

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

Opublikowane w: Environmental Pollution, Numer Volume 292, Part B, 1 January 2022, 118413, 2022, ISSN 0269-7491
Wydawca: Pergamon Press Ltd.
DOI: 10.1016/j.envpol.2021.118413

"""Systems toxicology to advance human and environmental hazard assessment: A roadmap for advanced materials"""
Autorzy: 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
Opublikowane w: Nano Today, Numer 48 (February 2023), 2023, ISSN 1748-0132
Wydawca: 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
Autorzy: Fan Zhang, Zhuang Wang, Martina G. Vijver, Willie J.G.M. Peijnenburg
Opublikowane w: Ecotoxicology and Environmental Safety, Numer Volume 219, August 2021, 112357, 2021, ISSN 1090-2414
Wydawca: 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)
Autorzy: Susana I. L. Gomes; Mónica J. B. Amorim; Suman Pokhrel; Lutz Mädler; Matteo Fasano; Eliodoro Chiavazzo; Pietro Asinari; Jaak Jänes; Kaido Tämm; Jaanus Burk; Janeck J. Scott-Fordsmand
Opublikowane w: Nanoscale, Numer 35/2021, 2021, ISSN 2040-3372
Wydawca: Royal Society of Chemistry
DOI: 10.1039/d1nr03231c

BMDx: a graphical Shiny application to perform Benchmark Dose analysis for transcriptomics data
Autorzy: Angela Serra, Laura Aliisa Saarimäki, Michele Fratello, Veer Singh Marwah, Dario Greco
Opublikowane w: Bioinformatics, Numer Volume 36, Numer 9, 2020, ISSN 1367-4811
Wydawca: Oxford University Press
DOI: 10.1093/bioinformatics/btaa030

Pulmonary toxicity of silver vapours, nanoparticles and fine dusts: A review
Autorzy: Niels Hadrup, Anoop K. Sharma, Katrin Loeschner, Nicklas R. Jacobsen
Opublikowane w: Regulatory Toxicology and Pharmacology, Numer 115, 2020, Strona(/y) 104690, ISSN 0273-2300

Wydawca: Academic Press
DOI: 10.1016/j.yrtph.2020.104690

Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields
Autorzy: Brajesh Narayan; Colm Herbert; Brian J. Rodriguez; Bernard R. Brooks; Nicolae-Viorel Buchete
Opublikowane w: The Journal of Physical Chemistry. B, Numer 125, 20, 2021, Strona(/y) 5233–5242, ISSN 1089-5639
Wydawca: American Chemical Society
DOI: 10.1021/acs.jpcb.1c01939

Trophic transfer of Cu nanoparticles in simulated aquatic food chains
Autorzy: Qi Yu, Zhuang Wang, Willie J. G. M. Peijnenburg, Martina G. Vijver
Opublikowane w: Ecotoxicology and Environmental Safety, Numer Volume 242, 1 September 2022, 113920, 2022, ISSN 1090-2414
Wydawca: Orlando, Fla. Academic Press
DOI: 10.1016/j.ecoenv.2022.113920

A systematic quality evaluation and review of nanomaterial genotoxicity studies – a regulatory perspective
Autorzy: Siivola KM, Burgum MJ, Suárez-Merino B, Clift M, Doak S and Catalán J
Opublikowane w: Particle and Fibre Toxicology, Numer 2022; 19: 59, 2022, ISSN 1743-8977
Wydawca: BioMed Central
DOI: 10.1186/s12989-022-00499-2

Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning
Autorzy: Brajesh Narayan; Nicolae-Viorel Buchete; Ron Elber
Opublikowane w: Jorunal of Physical Chemistry B, 2021, ISSN 1089-5639
Wydawca: American Chemical Society
DOI: 10.1021/acs.jpcb.1c00264

Core, Coating, or Corona? The Importance of Considering Protein Coronas in nano-QSPR Modeling of Zeta Potential.
Autorzy: Selvaraj Sengottiyan, Alicja Mikolajczyk, Karolina Jagiełło, Marta Swirog, and Tomasz Puzyn
Opublikowane w: ACS Nano, Numer Vol 17, Numer 3, 2023, ISSN 1936-0851
Wydawca: American Chemical Society
DOI: 10.1021/acsnano.2c06977

Assembling Biocompatible Polymers on Gold Nanoparticles: Towards a Rational Design of Particle Shape by Molecular Dynamics

Autorzy: Roberta Cappabianca, Paolo De Angelis, Annalisa Cardellini, Eliodoro Chiavazzo and Pietro Asinari
Opublikowane w: ACS Omega, Numer 2022, 7, 46, 2022, ISSN 2470-1343
Wydawca: ACS Publications
DOI: 10.1021/acsomega.2c05218

PROTEOMAS: a workflow enabling harmonized proteomic meta-analysis and proteomic signature mapping
Autorzy: Aileen Bahl, Celine Ibrahim, Kristina Plate, Andrea Haase, Jörn Dengjel, Penny Nymark & Verónica I. Dumit
Opublikowane w: Journal of Cheminformatics, Numer 15, Article number:34, 2023, ISSN 1758-2946
Wydawca: 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
Autorzy: Warisa Bunmahotama, Martina G. Vijver, Willie Peijnenburg
Opublikowane w: Environmental Toxicology and Chemistry, Numer 2022 Jun; 41(6): 1439–1450., 2022, ISSN 1552-8618
Wydawca: Society of Environmental Toxicology and Chemistry
DOI: 10.1002/etc.5322

Multi-Scale Modelling of Aggregation of TiO2 Nanoparticle Suspensions in Water
Autorzy: G.Mancardi(POLITO), M.Alberghini(POLITO), N.Aguilera-Porta(Sorbonne), M.Calatayud(Sorbonne), P.Asinari(POLITO&INRIM) and E.Chiavazzo(POLITO)
Opublikowane w: nanomaterials, Numer 2(2), 217, 2022, ISSN 2079-4991
Wydawca: MDPI
DOI: 10.3390/nano12020217

multiGSEA: a GSEA-based pathway enrichment analysis for multi-omics data.
Autorzy: Sebastian Canzler; Jörg Hackermüller
Opublikowane w: BMC Bioinformatics, Numer 21/2020, 2020, ISSN 1471-2105
Wydawca: BioMed Central
DOI: 10.1186/s12859-020-03910-x

Meta-analysis of Bioaccumulation Data for Nondissolvable Engineered Nanomaterials in Freshwater Aquatic Organisms
Autorzy: Yuanfang Zheng; Bernd Nowack
Opublikowane w: Environmental Toxicology and Chemistry, Numer Volume 41, Numer 5, 2022, Strona(/y) Pages 1202-1214, ISSN 1552-8618
Wydawca: SETAC
DOI: 10.1002/etc.5312

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

Autorzy: Vera L. Maria; David Licha; Janeck J. Scott-Fordsmand; Christian G. Huber; Mónica J.B. Amorim
Opublikowane w: Environmental Pollution, Numer 286, 2021, ISSN 1873-6424
Wydawca: Elsevier
DOI: 10.1016/j.envpol.2021.117571

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

Autorzy: Susana I.L. Gomes, Janeck J. Scott-Fordsmand and Monica J.B. Amorim
Opublikowane w: Nano Today, Numer Volume 40, October 2021, 101242, 2021, ISSN 1748-0132
Wydawca: 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)

Autorzy: Fátima C.F. Santosa, Rudo A. Verweijb, Cornelis A.M. van Gestelb and Mónica J.B. Amorima
Opublikowane w: Ecotoxicology and Environmental Safety, Numer Volume 252, 1 March 2023, 114599, 2023, ISSN 0147-6513
Wydawca: Academic Press
DOI: 10.1016/j.ecoenv.2023.114599

Graphene nanoplatelets and reduced graphene oxide elevate the microalgal cytotoxicity of nano-zirconium oxide.

Autorzy: Zhuang Wang; Fan Zhang; Martina G. Vijver; Willie J.G.M. Peijnenburg
Opublikowane w: Chemosphere, Numer 276, 2021, ISSN 1879-1298
Wydawca: Elsevier
DOI: 10.1016/j.chemosphere.2021.130015

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

Autorzy: Rita C. Bicho, Dick Roelofs, Janine Mariën, Janeck J. Scott-Fordsmand, Mónica J.B. Amorim
Opublikowane w: Environment International, Numer 136, 2020, Strona(/y) 105447, ISSN 0160-4120
Wydawca: Pergamon Press Ltd.
DOI: 10.1016/j.envint.2019.105447

Aquatic Mesocosm Strategies for the Environmental Fate and Risk Assessment of Engineered Nanomaterials.

Autorzy: Andrea Carboni; Danielle L. Slomberg; Mohammad Nassar; Catherine Santaella; Armand Masion; Jérôme Rose; Mélanie Auffan
Opublikowane w: https://hal-cnrs.archives-ouvertes.fr/hal-03468409, Numer 2, 2021, ISSN 0013-936X
Wydawca: American Chemical Society
DOI: 10.1021/acs.est.1c02221

Comparison of Biokinetic Models for Non-dissolvable Engineered Nanomaterials in Freshwater Aquatic Organisms
Autorzy: Yuanfang Zheng, Bernd Nowack
Opublikowane w: Environmental Science: Nano, Numer 2023,10, 1065-1076, 2023, ISSN 2051-8161
Wydawca: Royal Society of Chemistry
DOI: 10.1039/d2en01039a

Multivariate analysis of the exposure and hazard of ceria nanomaterials in indoor aquatic mesocosms
Autorzy: Mohammad Nassar; Mélanie Auffan; Mélanie Auffan; Catherine Santaella; Armand Masion; Jérôme Rose; Jérôme Rose
Opublikowane w: Environmental Science Nano, Numer 6/2020, 2020, ISSN 2051-8161
Wydawca: 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
Autorzy: Ankush Singhal; Geert Jan Agur Sevink
Opublikowane w: Nanoscale Advances, Numer 23/2021, 2021, ISSN 2516-0230
Wydawca: Royal Society of Chemistry
DOI: 10.1039/d1na00578b

Your Spreadsheets Can Be FAIR: A Tool and FAIRification Workflow for the eNanoMapper Database
Autorzy: Nikolay Kochev, Nina Jeliazkova, Vesselina Paskaleva, Gergana Tancheva, Luchesar Iliev, Peter Ritchie, Vedrin Jeliazkov
Opublikowane w: Nanomaterials, Numer 10/10, 2020, Strona(/y) 1908, ISSN 2079-4991
Wydawca: 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
Autorzy: Marta Swirog, Alicja Mikołajczyk, Karolina Jagiello, Jaak Jänes, Kaido Tämm, Tomasz Puzyn

Opublikowane w: Science of the Total Environment, Numer Volume 840, 20 September 2022, 156572, 2022, ISSN 1879-1026
Wydawca: Elsevier
DOI: 10.1016/j.scitotenv.2022.156572

Multigenerational Exposure to WCCo Nanomaterials—Epigenetics in the Soil Invertebrate Enchytraeus crypticus
Autorzy: Rita C. Bicho, Janeck J. Scott-Fordsmand, Mónica J.B. Amorim
Opublikowane w: Nanomaterials, Numer 10/5, 2020, Strona(/y) 836, ISSN 2079-4991
Wydawca: MDPI
DOI: 10.3390/nano10050836

How Does the Study MD of pH-Dependent Exposure of Nanoparticles Affect Cellular Uptake of Anticancer Drugs?
Autorzy: Selvaraj Sengottiyan, Alicja Mikolajczyk, Tomasz Puzyn
Opublikowane w: International Journal of Molecular Sciences, Numer Vol 24, Numer 4, 2023, ISSN 1422-0067
Wydawca: Multidisciplinary Digital Publishing Institute (MDPI)
DOI: 10.3390/ijms24043479

Materiały z konferencji (1)

"""Fostering EU-US Cooperation in Nanosafety"""
Autorzy: Miguel Bañares
Opublikowane w: 2019
Wydawca: Harvard University

Zbiory danych

Zbiory danych za pośrednictwem OpenAIRE (2)

ss-PDMFA: size-specific, probabilistic, dynamic material flow analysis
Autorzy: Zheng Yuanfang; Nowack Bernd
Opublikowane w: Zenodo

Classification of GTP-dependent K-Ras4B active and inactive conformational states

Autorzy: Narayan, Brajesh; Kiel, Christina; Buchete, Nicolae-Viorel
Opublikowane w: Zenodo

Pozostałe produkty badawcze

Pozostałe produkty badawcze dostępne przez OpenAire (1)

Data & code repository for the article "An ancestral molecular response to nanomaterial particulates"

Autorzy: Giudice, Giusy Del; Greco, Dario
Opublikowane w: Zenodo

Ostatnia aktualizacja: 11 Grudnia 2023

Permalink: https://cordis.europa.eu/project/id/814426/results/pl