







NanoInformaTIX the value of data



Despite the considerable amount of data from experimental studies on the potential (eco)-toxicity of engineered nanomaterials (ENM) in new products, we still need reliable infomatics tools for modeling the risk linked to engineered nanomaterials

NanoInformaTIX will develop, validate and implement a Sustainable NanoInformatics Framework (SNF) for the risk assessment of ENM and for informing safer design of quality products









THE VALUE OF DATA

DATA

- 1. From completed EU projects (e.g. MARINA, NanoVALID, NanoSOLUTIONS, SUN, etc.) and established databases (e.g. eNanoMapper, DaNA and NanoWerk);
- Emerging data from ongoing projects (NanoReg², CaliBRATE, PATROLS, GRACIOUS, BIORIMA);
- 3. North American projects (e.g. from NIOSH, UCLA, Duke University and Health Canada); Chinese projects (from the Chinese Academy of Sciences); South African projects (from MinTek) and curated peer reviewed literature.

OECD validation principles

Materials modelling Exposure modelling Bio-distribution modelling Dose-Response modelling

MODELS

NanoInformaTIX will develop and extend existing models - some created in recent modelling projects (NanoSOLUTIONS, MOD-ENP-TOX, MODERN, PRENANOTOX, MEMBRANENANOPART, NANOPUZZLES and the COST Action TD1204 MODENA) or projects with a modelling component (e.g. ENPRA, MARINA).

SNF will be co-implemented together with **stakeholders** to ensure a user-friendly interface for industry, regulators, researchers and civil society, providing costeffective safety assessment guidance.









OBJECTIVES

Database

the database will be implemented by collecting and managing data from existing EU/US Canada/China completed and ongoing projects

Material Modelling

develop multiscale, bottom up methods to ENM design; model advanced descriptors; implement a 'Safe-by-Design' approach. Both specific functionalities and hazard will be predicted

Fate-Exposure Modelling

develop models of ENM exposure including models of ENM release, fate and environmental distribution; models of ENM bio-distribution using PBPK, linking the ENM descriptors to their pharmacokinetics

Dose-Response Modelling

Use top-down data mining, QSAR methods and other quantitative methods to derive models of the ENM dose-response relationship for (eco)-toxicity, allowing ENM descriptors to be linked to adverse outcomes

Integration/linking of Models

Chain data sources and models to enable specific operations needed for risk assessment (e.g. *in vitro-in vivo* extrapolation, dose-response assessment, grouping, readacross) as well as predictions of properties and effects for safer design of quality products

Model validation

Improve model prediction using the advanced descriptors ; validate the models by comparing model predictions with data from completed and currently ongoing EU and national projects

Sustainable NanoInformatics Framework

web-based software platform





>_NanoInformaTIX will bring predictive toxicology knowledge to enable engineered nanomaterials (ENM) sustainable production through:

- \checkmark reduction of animal experimentation
- ✓ Safe-by-Design
- ✓ Grouping/classifying for risk assessment of ENM

>_The SNF will become a **global hub for ENM safe-by-design**, a portal for manufacturers and scientists to go to for information on their materials.

>_The SNF enabling technology will help shortening considerably the path from lab bench to the market offering a **tangible product that can be used and upgraded in the future**.













Industry

speed, cost-effective production, use of safe-by-design which anticipates uncertainties and risks early in the innovation process, helping industries to be more competitive

MM

Consumers

safer and better products on the market, transparency and trust



Regulators

sound, validated methodologies



availability of tools to turn research into successful products



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METHODOLOGY

- >_WP1_ Project management and Coordination
- >_WP2_Data and database
- >_WP3_Nanomaterials and Material Modelling
- >_WP4_Exposure and Bio-Distribution Modelling
- >_WP5_Dose-Response Modelling
- >_WP6_Model validation and integration
- >_WP7_ Implementation of a sustainable

SNF Platform

>_ WP8_Dissemination, Exploitation, Training





WP8 Task 8.1 Dissemination and Communication; Task8.2 Training; T8.3 Development of the plan for sustainability









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PROJECT INFO



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> TITLE Development and Implementation of a

Sustainable Modelling Platform

for NanoInformatics

- > ACRONYM NanoInformaTIX
- START/END Jan 2019 Feb 2023
- > DURATION 50 months
- > TOTAL COST EUR 7,751,271.25
- > EU CONTRIBUTION EUR 6,783,556.25
- > TOPIC NMBP-14-2018
- > PROJECT REFERENCE 814426
- >_ 36 partners from 18 European Countries
- + 4 International (South Africa, China, Taiwan, Israel)

www.nanoinformatix.eu









MORE INFO



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