



# Nanosafety Cluster Annual Conference 2019

## Towards in silico nanosafety assessment – integrating experimental and computational approaches

Conference venue: Eigtveds Pakhus, Strandgade 25G, 1401 København. <https://um.dk/da/om-os/kontakt/eigtveds-pakhus/find-os/>

Tuesday 8 <sup>th</sup> October		
09.00 – 09.05	Welcome and Conference opening	
09.05 – 10.05	<b>Keynote Session 1 – Introduction to the organising and sponsoring projects</b> NanoSolveIT - Antreas Afantitis NanoInformaTIX – Miguel Banares NanoCommons – Iseult Lynch CaLIBRAte – Keld Alstrup Jensen	
10.05 – 10.30	<b>Plenary 1: Pietro Asinari</b> (Politecnico di Torino) “The role of materials modelling in nanosafety assessment”	
10.30 -11.00	<b>Morning Coffee</b>	
<b>Parallel sessions 1</b>	<b>Systems biology &amp; mechanistic insights for nanosafety</b> <i>Co-Chairs:</i> Dario Greco and Jaanus Burk	<b>Hazard assessment along the life cycle of nanomaterials and nano-enabled products</b> <i>Co-Chairs:</i> Panagiotis Isgonis and Tassos Papadiamantis
11.00 – 11.15	Characterisation of the Mechanism of Action of MWCNT by Integrated Modelling of Time- and Dose-Dependent Molecular Alterations - <i>Laura Aliisa Saarimäki</i> (Tampere University)	Toxicity and bioavailability of different forms of copper and copper nanoparticles to the earthworm <i>E. fetida</i> - <i>David Spurgeon</i> (UKRI Centre for Ecology & Hydrology)
11.15 – 11.30	An integrative computational approach for prioritization of key transcription regulators associated with nanomaterial-induced toxicity – <i>Vadim Zhernovkov</i> (University College Dublin)	Pulmonary toxicity of silica nanomaterials - effects of porosity and copper doping - <i>Niels Hadrup</i> (National Research Centre for the Working Environment)
11.30 – 11.45	Common gene expression patterns in environmental model organisms exposed to engineered nanomaterials: a meta-analysis - <i>Michael Burkard</i> (Eawag)	Amino functionalization of nanodiamonds reduces their toxic effects on human immune cells ex vivo - <i>Lucia Gemma Delogu</i> (University of Trieste)
11.45 – 12.00	R based Shiny software suite for transcriptomic analyses in toxicogenomics - <i>Angela Serra</i> (Tampere University)	Silver nanoparticles absorption through oromucosal barrier: differences between adult and young tissue - <i>Marcella Mauro</i> (University of Trieste)
<b>12.00 – 13.00</b>	<b>Lunch</b>	
<b>13.00 – 13.30</b>	<b>Plenary 2: Antreas Afantitis/ Philip Doganis</b> “The NanoSolveIT Cloud platform for Chemical/Nano-safety, Environmental Science and Pharmacokinetics”	
<b>Parallel sessions 2</b>	<b>NanoInformatics and Predictive Modelling</b> <i>Co-Chairs:</i> Antreas Afantitis and Pietro Asinari	<b>Exposure assessment along the life cycle of nanomaterials and nano-enabled products</b> <i>Co-Chairs:</i> Keld Aastrup and Wouter Fransman

13.30 – 13.45	<i>In silico</i> characterization of nanomaterials for predictive toxicology – <i>Vladimir Lobaskin</i> (University College Dublin)	Occupational exposure and environmental release: The case study of pouring TiO <sub>2</sub> and filler materials for paint production - <i>Ana Sofia Fonseca</i> (National Research Centre for the Working Environment)
13.45– 14.00	Towards integrating Nano-QSAR and Nano-AOP - <i>Karolina Jagiello</i> (QSAR Lab Ltd.)	Physicochemical analysis of chemical surface modifications – a case study on particle aging under real-life conditions - <i>Mark Geppert</i> (Paris Lodron University of Salzburg)
14.00 – 14.15	Jaqpot - An open-source web platform for creating, using, testing and sharing predictive models in nano-informatics within the NanoCommons KnowledgeBase - <i>Philip Doganis</i> (National Technical University Of Athens)	Safety Observer app template for use in measuring safe and healthy working conditions and behaviour with nanomaterials - <i>Pete Kines</i> (National Research Centre for the Working Environment)
14.15 – 14.30	Development and utilization of full-particle nanodescriptors - <i>Jaanus Burk</i> (UppinTech OÜ)	Inventory and Gap analysis - <i>Arto Saamanen</i> (Finnish Institute of Occupational Health)
14.30 – 14.45	Predictive toxicogenomics space modelling explores adverse outcomes of nanomaterials by omics-driven informatics - <i>Roland Grafström</i> (Misvik Biology)	Refining an integrative model for predicting environmental emissions of engineered nanomaterials - <i>Vicenç Pomar-Portillo</i> (LEITAT)
14.45 – 15.00	A higher-tier model for fate, speciation and biouptake of nanomaterials in the environment - <i>Sam Harrison</i> (Centre for Ecology & Hydrology)	Nanowaste and Regulation: (In)-significant challenges for treatment and recycling? - <i>Tobias Walser</i> (Vereala GmbH)
<b>15.00 – 15.30</b>	<b>Afternoon tea</b>	
<b>Parallel sessions 3</b>	<b>Tools and approaches for safe by design of nanomaterials and processes</b> <i>Co-Chairs: Vladimir Lobaskin and Iseult Lynch</i>	<b>Hazard assessment along the life cycle of nanomaterials and nano-enabled products (Continued)</b> <i>Co-Chairs: Roland Grafström and Neil Hunt</i>
15.30 - 15.45	Ensembles, comparison and ranking of nanoparticles toxicity classifiers: a hands-on paradigm on the S2NANO database - <i>Irini Furxhia</i> (University of Limerick)	Silver nanoparticles toxicity and cell death mechanisms in Zebrafish Cells - <i>Ana Carrasco-Quevedo</i> (University of Birmingham)
15.45 – 16.00	Exploring the complete corona of nanomaterials – the interplay between the small molecule and proteins coronas – <i>Andrew Chetwynd</i> (University of Birmingham)	Effect of porosity and copper doping on the in vivo genotoxic response of silica nanoparticles – <i>Julia Catalan</i> (Finnish Institute of Occupational Health)
16.00 – 16.15	Guidelines to implement a Safe-by-Design approach for medicinal polymeric nanobiomaterials - <i>Mélanie Schmutz</i> (Empa)	A potential integrated pathway for an early in vitro-based hazard assessment of nanoparticles - <i>Daina Romeo</i> (Empa)
16.15 – 16.30	Testing and demonstrating of the sensor dish reader™ method for screening and ranking of nanomaterials reactivity and solubility - <i>Amalie Kofoed Jørgensen</i> (National Research Centre for the Working Environment)	Interaction of graphene oxide with keratinocytes: The influence of protein corona on toxicity and secretomics - <i>Diego Martinez</i> (Brazilian Nanotechnology National Laboratory)
16.30 – 16.45	Towards a Sustainable European Centre for Risk Management and Safe Innovation in Nanomaterials and Nanotechnologies – <i>Effie Marcoulaki</i> (Demokritos)	Predictive 3D lung models to assess the long-term hazard of nanomaterial aerosols - <i>Kirsty Meldrum</i> (Swansea University Medical School)
16.45 – 17.00	<b>Speed introduction to posters (1 slide / 1 minute)</b>	
<b>17.00 – 19.00</b>	<b>Poster session with drinks and finger food</b> <b>NanoCommons Transnational Access poster corner</b>	
<b>Wednesday 9<sup>th</sup> October</b>		
<b>9.00 – 9.30</b>	<b>Plenary 3: Maria Dusinska</b> (NILU) “Risk Governance of Nanomaterials - 3 European Projects Working Together”	
<b>Topic 4</b>	<b>Categorisation &amp; grouping of nanomaterials</b>	<b>Risk assessment and risk management solutions</b>

	<i>Co-Chairs: Dave Spurgeon and Gianpietro Basei</i>	<i>Co-Chairs: Andrea Haase and Flemming Cassee</i>
09.30 – 09.45	Assessment of Cytotoxicity of Metal Oxide Nanoparticles on the Basis of Fundamental Physical-Chemical Parameters: a Robust Approach to Grouping - <i>Felice Simeone</i> (National Research Council of Italy)	Transferring Best Practices from Nanomaterial Risk Analysis to Other Emerging Technologies - <i>Khara Grieger</i> (North Carolina State University)
09.45 – 10.00	Dissolution behaviour of a library of 37 nanomaterials in simplified physiological media - <i>Anastasios Papadiamantis</i> (UoB)	Data to support Risk Assessment along use-phase and end-of-life: the caLIBRAte case study on paints containing TiO <sub>2</sub> and filler materials - <i>Camilla Delpivo</i> (LEITAT Technological Center)
10.00 – 10.15	SimpleBox4nano: Screening level multimedia fate model for engineered nanomaterials - <i>Joris Quik</i> (National Institute for Public Health and the Environment)	Towards the development of a community-based state-of-the-art Risk Assessment toolbox within the NanoCommons Knowledge base - <i>Philip Doganis</i> (National Technical University Of Athens)
10.15 – 10.30	A comparison of acellular methods for assessing reactive oxygen species produced by nanomaterials – efficient risk assessment by applying grouping approaches - <i>Matthew Boyles</i> (IOM)	The Precautionary Matrix for Nanomaterials: A Predictive Tool for Risk Estimation beyond single Life Cycle Stages - <i>Tobias Walser</i> (Vereala GmbH)
<b>10.30 -11.00</b>	<b>Coffee</b>	
11.00 – 11.15	The GRACIOUS draft Framework for the Grouping of Nanomaterials in order to streamline risk assessment and decision making - <i>Neil Hunt</i> (Yordas Group)	Risk management framework for nano-biomaterials used in medical devices and advanced therapy medicinal products – <i>Virginia Cazzagon</i> (University Ca' Foscari of Venice)
11.15 – 11.30	The ten decrees of nanomaterials regulations - <i>Steffen Foss Hansen</i> (Technical University of Denmark)	Prioritizing New Approach Methodologies for Safety Assessment along the Stage-Gate Innovation Funnel - <i>Penny Nymark</i> (Karolinska Institutet)
11.30 – 11.45	High-throughput hazard-based scoring, ranking and grouping of engineered nanomaterials - <i>Vesa Hongisto</i> (Misvik Biology Oy)	Criteria and tools for risk evaluation, mitigation and communication, the implementation of which can inform better risk management decision making - <i>Panagiotis Isigonis</i> (University Ca' Foscari of Venice)
11.45 – 12.00	NanoExplore - Integrated approach for exposure and health effects monitoring of engineered nanomaterials in workplaces and urban areas - <i>Eva Penssler</i> (Yordas Group)	EC4SafeNano: Visions for Global Networking - <i>Anna-Kaisa Viitanen</i> (Finnish Institute of Occupational Health, Helsinki)
12.00 – 12.30	<b>Plenary 4: Thomas Exner</b> (Edelweiss Connect GmbH) “The NanoCommons knowledge infrastructure built to support the research communities, industrial users and regulators in the area of nanomaterials safety assessment”	
<b>12.30 – 13.30</b>	<b>Lunch</b>	
	<b>Nanosafety Data Management Tools</b> <i>Co-Chairs: Antreas Afantitis and Effie Marcoulaki</i>	
13.30 – 13.45	caLIBRAte: Collecting data fit for purpose - <i>Martine Bakker</i> (National Institute of Public Health and the Environment)	
13.45 – 14.00	ACEnano knowledge infrastructure to support data collection, methods optimisation and knowledge sharing in the area of physicochemical characterisation of nanomaterials - <i>Thomas Exner</i> (Edelweiss Connect GmbH)	
14.00 – 14.15	Nanomaterial safety data integration with eNanoMapper database - <i>Nikolay Kochev</i> (Ideaconsult Ltd.)	
14.15 – 14.30	Towards a decision support infrastructure for the safety assessment of engineered nanomaterials used in consumer products and medical technologies - <i>Alex Zabeo</i> (GreenDecision s.r.l.)	

14.30 – 14.45	The NanoInformaTIX Sustainable Data and Modelling Platform - <i>Gianpietro Basei</i> (Greendecision Srl.)	
14.45 – 15.00	Closing remarks and best oral & poster award. Launch of the NanoCommons curation award.	
<b>15.00 – 15.30</b>	<b>Closing of the Conference and Afternoon tea</b>	
<b>15.30 – 18.00</b>	<b>NanoSafety Cluster Steering Group Meeting</b> (closed meeting)	

## List of poster presentations

1. Prediction of Nanomaterial Cytotoxicity through Application of Machine Learning Algorithms - *Mohammad Zein Aghaji* (Health Canada)
2. Development of nanodescriptors and modelling of toxicities of Fe doped ZnO nanoparticles - Kaido Tamm, Jaanus Burk (UppinTech OÜ) and Jaak Jänes (University of Tartu)
3. DaNa2.0 Knowledge Base - Quality-approved information on Safety of Nanomaterials from experts for the public – *Clarissa Marquardt* (Karlsruhe Institute of Technology)
4. Comparison of SSD models for environmental risk assessment of nanomaterials – a case study - *Sara Nørgaard Sørensen* (Technical University of Denmark)
5. Compilation of suitable value-chain case-studies to complete demonstration of the caLIBRAte Nano-Risk Governance framework - *Camilla Delpivo* (LEITAT Technological Center)
6. Value-chain case-studies for models performance testing in caLIBRAte project - *Ana Sofia Fonseca* (National Research Centre for the Working Environment)
7. Occupational Exposure Modelling Tools: requirements and lessons learned - *Ana Sofia Fonseca* (National Research Centre for the Working Environment)
8. PATROLS: Physiologically Anchored Tools for Realistic nanomaterial hazard assessment – *Claire Skentlebery* (Nanomaterials Industry Association)
9. Development, characterization and evaluation of 3D liver models for in vitro Engineered Nanomaterial toxicology testing - *Kirsty Meldrum* (Swansea University Medical School)
10. Development of multicellular 3D in vitro models of the gut and their application in the hazard assessment of engineered nanomaterials - *Kirsty Meldrum* (Swansea University Medical School)
11. GRACIOUS Wiki and Blueprint - *Alex Zabeo* (Greendecision Srl.)
12. Use of human 3D models in Nanotoxicology and its applications in risk assessment - *Isabel Rodriguez-Llopis* (GAIKER Technology Centre)
13. A new integration framework to ensure the safety and the sustainability of nanoproducts - *Beatrice Salieri* (Empa)
14. Decision tools for supporting risk-benefit analysis and safer innovation of nano-biomaterials used in the medical sector – *Lisa Pizzol* (GreenDecision s.r.l.)
15. What is the effect of porosity and copper doping on nanomaterial toxicity? - *Niels Hadrup* (on behalf of the caLIBRAte EU project)
16. Risk assessment of NECOMADA development process and pilot line - *Anna-Kaisa Viitanen* (Finnish Institute of Occupational Health)
17. Evaluation of the perception and knowledge of nanotechnology in the Austrian society - *Isabella Joubert* (University of Salzburg)
18. Physicochemical characteristics of synthesized non-porous and meso-porous silica materials, radical formation capacity and dissolution in Gambles solution - *N.M. Sahlgren* (NCRWE)
19. The non-canonical TFF2 /IL-33 pathway and fibrosis induced by asbestos-like fibers - *Henrik Wolff* (Finnish institute of Occupational Health)

### *NanoCommons Transnational Access poster session:*

20. Enalos Cloud Platform Transnational Access Services Through NanoCommons H2020 Infrastructure Project - *Georgia Melagraki* (Novamechanics Ltd.)
21. PBPK modelling on the Jaqpot web platform- a PAA-peg nanoparticles case study - *Philip Doganis* (National Technical University Of Athens)
22. H2020 NanoCommons Transnational Access Services: Data management in nanosafety research. From bench to database thus streamlining analysis and publication - *Anastasios G. Papadiamantis* (University of Birmingham)
23. NanoCommons - Opportunities for accessing nanoinformatics and predictive models for environment fate. *Lee A. Walker* (Centre for Ecology and Hydrology)
24. NanoCommons – Assistance with Data Management & Nanoinformatics Tools - *Beatriz Alfaro Serrano* (BioNanoNet)
25. NFFA-Europe: enhancing European competitiveness in nanoscience research and innovation – *Cecile Girardot* (European Synchrotron Radiation Facility)