



1st Interprofessional Nano Training School

Cutting Edge Approaches for the Risk Assessment and Management of Nano-(bio)materials: From the Lab to the Market

H2020 BIORIMA-GRACIOUS-NanoInformaTIX Training School

List of relevant references, publications and sources

Session 1 – Hazard to Human Health & Environment

Boyles MS, Young L, Brown DM, MacCalman L, Cowie H, Moisala A, Smail F, Smith PJ, Proudfoot L, Windle AH, Stone V. (2015) Multi-walled carbon nanotube induced frustrated phagocytosis, cytotoxicity and pro-inflammatory conditions in macrophages are length dependent and greater than that of asbestos. *Toxicol In Vitro*. 29(7):1513-28.

Brown DM, Kinloch IA, Bangert U, Windle AH, Walter DM, Walker GS, Scotchford CA, Donaldson K, Stone V. (2007). An in vitro study of the potential of carbon nanotubes and nanofibres to induce inflammatory mediators and frustrated phagocytosis. *Carbon*. 45:1743–1756.

Burden N, Aschberger K, Chaudhry Q, Clift MJD, Fowler P, Johnston H, Landsiedel R, Rowland J, Stone V, Doak SH. (2017) Aligning nanotoxicology with the 3Rs: What is needed to realise the short, medium and long-term opportunities? *Regul Toxicol Pharmacol*. 91:257-266.

Donaldson K, Murphy FA, Duffin R, Poland CA. (2010). Asbestos, carbon nanotubes and the pleural mesothelium: a review of the hypothesis regarding the role of long fibre retention in the parietal pleura, inflammation and mesothelioma. *Part Fibre Toxicol*. 7:5.

Donaldson K, Poland CA, Murphy FA, MacFarlane M, Chernova T, Schinwald A. (2013). Pulmonary toxicity of carbon nanotubes and asbestos - similarities and differences. *Adv Drug Deliv Rev*. 65(15):2078-86.

Johnston HJ, Verdon R, Gillies S, Brown DM, Fernandes TF, Henry TB, Rossi AG, Tran L, Tucker C, Tyler CR, Stone V. (2018). Adoption of in vitro systems and zebrafish embryos as alternative models for reducing rodent use in assessments of immunological and oxidative stress responses to nanomaterials. *Crit Rev Toxicol* 48(3):252-271.

Murphy FA, Poland CA, Duffin R, Al-Jamal KT, Ali-Boucetta H, Nunes A, Byrne F, Prina-Mello A, Volkov Y, Li S, Mather SJ, Bianco A, Prato M, Macnee W, Wallace WA, Kostarelos K, Donaldson K. (2011). Length-dependent retention of carbon nanotubes in the pleural space of mice initiates sustained inflammation and progressive fibrosis on the parietal pleura. *Am J Pathol*. 178(6):2587-600.

Murphy FA, Poland CA, Duffin R, Donaldson K. (2013). Length-dependent pleural inflammation and parietal pleural responses after deposition of carbon nanotubes in the pulmonary airspaces of mice. *Nanotoxicology*.7(6):1157-67.

Poland CA, Duffin R, Kinloch I, Maynard A, Wallace WA, Seaton A, Stone V, Brown S, Macnee W, Donaldson K. (2008) Carbon nanotubes introduced into the abdominal cavity of mice show asbestos-like pathogenicity in a pilot study. *Nat Nanotechnol*. 2008 Jul;3(7):423-8

OECD (2016). GUIDANCE DOCUMENT ON THE REPORTING OF DEFINED APPROACHES TO BE USED WITHIN INTEGRATED APPROACHES TO TESTING AND ASSESSMENT Series on Testing & Assessment No. 255. ENV/JM/MONO(2016)28.

Session 2 – Fate & Exposure Assessment

Som, C., Berges, M., Chaudhry, Q., Dusinska, M., Fernandes, T. F., Olsen, S. I., Nowack, B. (2010). The importance of life cycle concepts for the development of safe nanoproducts. *Toxicology* 269, 160-169.

Nowack, B., Brouwer, C., Geertsma, R. E., Eugens, E. H. W., Ross, B. L., Toufektsian, M. C., Wejnhoven, S. W. P., Aitken, R. J. (2013). Analysis of the occupational, consumer and environmental exposure to engineered nanomaterial used in 10 technology sectors. *Nanotoxicology* 7(6):1152-1156.

Session 3 – Nanomedicine: from the lab to the market

Salvati et al, 2013, Transferrin-functionalized nanoparticles lose their targeting capabilities when a biomolecule corona adsorbs on the surface, *Nature Nanotechnology*.

Wilhelm, S. et al., 2016, Analysis of nanoparticle delivery to tumours. *Nat. Rev. Mater.*, doi: 10.1038/natrevmats.2016.14.

Ledford H. Bankruptcy of nanomedicine firm worries drug developers. *Biotechnology*. 2016.

Bourzac, 2016, Cancer nanomedicine, reengineered, *PNAS*, doi: 10.1073/pnas.1616895113.

Van der Meel et al., 2017, Cancer nanomedicines: oversold or underappreciated, *Expert Opinion on Drug Delivery*, doi: 10.1080/17425247.2017.1262346.

Halappanavar et al., 2018, Promise and peril in nanomedicine: the challenges and needs for integrated systems biology approaches to define health risk, *WIREs Nanomed Nanobiotechnol*, doi: 10.1002/wnan.1465.

Session 4 – Modelling

Transcriptomics data preprocessing and analysis

Marwah, V. S., Scala, G., Kinaret, P. A. S., Serra, A., Alenius, H., Fortino, V., & Greco, D. (2019). eUTOPIA: solUTion for Omics data Preprocessing and Analysis. *Source code for biology and medicine*, 14(1),.

Veer Singh Marwah, Pia Anneli Sofia Kinaret, Angela Serra, Giovanni Scala, Antti Lauerma, Vittorio Fortino, Dario Greco; INfORM: Inference of NetwOrk Response Modules, *Bioinformatics*, Volume 34, Issue 12, 15 June 2018, Pages 2136–2138.

Scala G, Serra A, Marwah VS, Saarimäki LA, Greco D. FunMappOne: a tool to hierarchically organize and visually navigate functional gene annotations in multiple experiments. *BMC Bioinformatics*. 2019 Feb 15;20(1):79. doi: 10.1186/s12859-019-2639-2. PubMed PMID: 30767762; PubMed Central PMCID: PMC6376640.

Kinaret P, Marwah V, Fortino V, Ilves M, Wolff H, Ruokolainen L, Auvinen P, Savolainen K, Alenius H, Greco D. Network Analysis Reveals Similar Transcriptomic Responses to Intrinsic Properties of Carbon Nanomaterials in Vitro and in Vivo. *ACS Nano*. 2017 Apr 25;11(4):3786-3796. doi: 10.1021/acsnano.6b08650. Epub 2017 Apr 11. PubMed PMID: 28380293.

Scala, G, Kinaret, P, Marwah, V, Sund, J, Fortino, V & Greco, D 2018 'Multi-omics analysis of ten carbon nanomaterials effects highlights cell type specific patterns of molecular regulation and adaptation', *NanoImpact*, vol. 11, pp. 99-108.



Serra, A., Letunic, I., Fortino, V., Handy, R. D., Fadeel, B., Tagliaferri, R., & Greco, D. (2019). INSIDE NANO: a systems biology framework to contextualize the mechanism-of-action of engineered nanomaterials. *Scientific reports*, 9(1), 179.

QSAR modeling

Mikolajczyk et al. Zeta Potential for Metal Oxide Nanoparticles: A Predictive Model Developed by a Nano-Quantitative Structure–Property Relationship Approach, *Chem. Mater.* 2015, 27, 7, 2400-2407

Mikolajczyk et al. Nano-QSAR modeling for ecosafe design of heterogeneous TiO₂-based nanophotocatalysts, *Environ. Sci.: Nano*, 2018, 5, 1150-1160

Puzyn et al. Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles, *Nature Nanotechnology*, 2011, 6, 175–178

Recommended software

R

RStudio software

Eutopia software: instruction on how to install it can be found here: <https://github.com/Greco-Lab/eUTOPIA>

INFORM software: instruction on how to install it can be found here: <https://github.com/Greco-Lab/INFORM>

Latex system libraries

Java

Session 5 – Grouping & Read Across Approaches

Lamon, L. et al. Grouping of nanomaterials to read-across hazard endpoints: from data collection to assessment of the grouping hypothesis by application of chemoinformatic techniques. *Part. Fibre Toxicol.* 15, 37 (2018).

Appendix X in Worth et al., "Evaluation of the availability and Worth applicability of computational approaches in the safety assessment of nanomaterials", EUR 28617 EN, Publications Office of the European Union, Luxembourg, 2017, doi: 10.2760/248139A

<http://publications.jrc.ec.europa.eu/repository/bitstream/JRC106386/kjna28617enn.pdf>

Lamon, L., Aschberger, K., Asturiol, D., Richarz, A. & Worth, A. Grouping of nanomaterials to read-across hazard endpoints: a review. *Nanotoxicology* 1–19 (2018). doi:10.1080/17435390.2018.1506060

ECHA. Appendix R . 6-1 : Recommendations for nanomaterials applicable to the Guidance on QSARs and Grouping. (2017). doi:10.2823/884050

Mech A. et al. Insights into possibilities for Grouping and Read-Across for Nanomaterials in EU Chemicals Legislation. *Nanotoxicology*: 1-23 (2018). doi: 10.1080/17435390.2018.1513092.

eNanoMapper database:

<https://apps.ideaconsult.net/nanodata/index.html> (<https://search.data.enanomapper.net/nanoreg/>)

Session 6 – Risk Assessment & Management Strategies

<https://sunds.gd/>

<https://temas.taglab.ch/SbDimplementation/index.php?p=home>



Hristozov, D.; Pizzol, L.; Basei, G.; Zabeo, A.; Mackevica, A.; Hansen, S.F.; Gosens, I.; Cassee, F. R.; de Jong, W.; Koivisto, A. J.; Neubauer, N.; Sanchez Jimenez, A.; Semenzin, E.; Subramanian, V.; Fransman, W.; Jensen, K. A.; Wohlleben, W.; Stone, V.; & Marcomini, A. (2018). Quantitative human health risk assessment along the lifecycle of nano-scale copper-based wood preservatives. *Nanotoxicology* 12(7), pp. 747-765, doi: 10.1080/17435390.2018.1472314

Pizzol, L.; Hristozov, D.; Zabeo, A.; Basei, G.; Wohlleben, W.; Koivisto, A. J.; Jensen, K. A.; Fransman, W.; Stone, V.; & Marcomini, A. (2019). SUNDS probabilistic human health risk assessment methodology and its application to organic pigment used in the automotive industry. *NanoImpact*, 13, pp. 26-36.

Kraegeloh, A., Suarez-Merino, B., Sluijters, T., & Micheletti, C. (2018). Implementation of Safe-by-Design for Nanomaterial Development and Safe Innovation: Why We Need a Comprehensive Approach. *Nanomaterials* (Basel, Switzerland), 8(4), 239. doi:10.3390/nano8040239