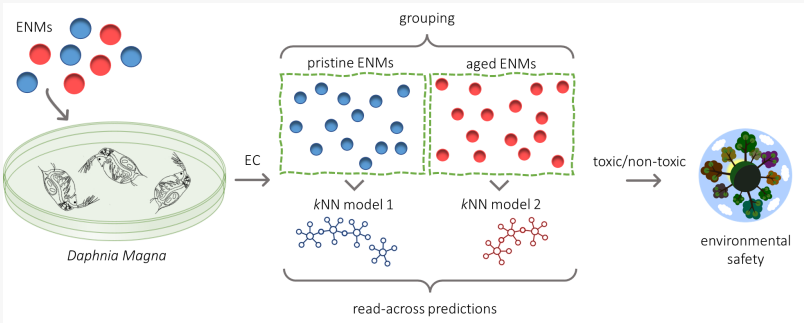
Is time spend in the environment a key toxicity factor in nanomaterials?

Researchers from NanoSolveIT H2020 nanoinformatics project developed ecotoxicological read-across models for predicting NMs acute toxicity,



Comparing the toxicity of freshly dispersed NMs with the same NMs stored for 2 years in artificial river waters of different composition to the water flea Daphnia magna.

CYRPUS, February 4, 2022 /EINPresswire.com/ -- It is almost 20 years since the commercialization of nanomaterials (NMs) started but there is still a long way to go to fully unravel their interactions with living organisms. A recent paper, published in Elsevier's Chemosphere (https://doi.org/10.1016/j.chemosphere.2021.131452) compares the toxicity of freshly dispersed NMs with the same NMs stored for 2 years in artificial river waters of different composition (environmentally aged NMs) to the water flea Daphnia Magna. Researchers assumed that the aged NMs might have different toxicity and they were proved right: NMs aged in both salt-only artificial river water and river water containing both salts and natural organic matter caused much less toxicity to the daphnids that the freshly dispersed NMs due to passivation of the surface reactivity over time.

> Nanoinformatics is an evolving field of research that includes the development of in silico models and tools that could be an alternative to the experimental evaluation of nanomaterials (NMs)."
>
> *Antreas Afantitis*

Researchers from NovaMechanics Ltd and the University of Birmingham developed ecotoxicological read-across models for predicting NMs acute toxicity, following the strategy recommended by the European Chemicals Agency for NMs grouping. The computational modeling procedure was performed by combining widely accepted and accurate informatics tools including the Isalos & KNIME Analytics Platforms with the Enalos Cloud Platform, which facilitates the manipulation of big data. The predictive power of the proposed Quantitative Structure-Activity Relationship (QSAR) models has been evaluated according to the criteria prescribed by the Organisation for Economic Cooperation and Development, and a QSAR Model Reporting Format (QMRF) report has been produced and made available in the supplementary

information of the paper to support regulatory acceptance and uptake. An additional important outcome of this study was the creation of Findable, Accessible, Interoperable and Reusable (FAIR) datasets that will help other scientists to further investigate and predict the toxicity of freshly dispersed and environmentally aged NMs.

Iseult Lynch, Professor of Environmental Nanosciences at the University of Birmingham notes that "The need to build reliable prediction models for NMs is often highlighted as a significant regulatory challenge, since it is not possible to experimentally assess all variants of NMs due to time, cost and ethical restrictions, and thus computational models utilizing regulatory-relevant species such as D. Magna that can predict the toxicity of data-poor NMs are urgently needed."

The newly developed nanoinformatics models, which help researchers to explore in silico the effects of a panel of freshly dispersed versus environmentally aged NMs, is an important advance. Antreas Afantitis, Managing Director of NovaMechanics Ltd (www.novamechanics.com) and NanoSolveIT (www.nanosolveit.eu) Project Coordinator highlights that "Nanoinformatics is an evolving field of research that includes the development of in silico models and tools that could be an alternative to the experimental evaluation of nanomaterials (NMs) environmental health and safety (exposure and toxicity) and thus contribute to NMs hazard and risk assessment."

The machine learning read across model is available through NanoSolveIT Cloud Platform (https://ecotox.cloud.nanosolveit.eu/) and the full dataset is available through the nanoPharos (2021) database https://db.nanopharos.eu/Queries/Datasets.zul) developed under the H2020 NanoSolveIT and NanoCommons projects, in compliance with the FAIR data principles and is ready for further computational analysis.

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