

NanoSolveIT H2020 project makes freely available a library of critical characteristics for 69 engineered nanomaterials

This is the fifth freely available application that the project delivers

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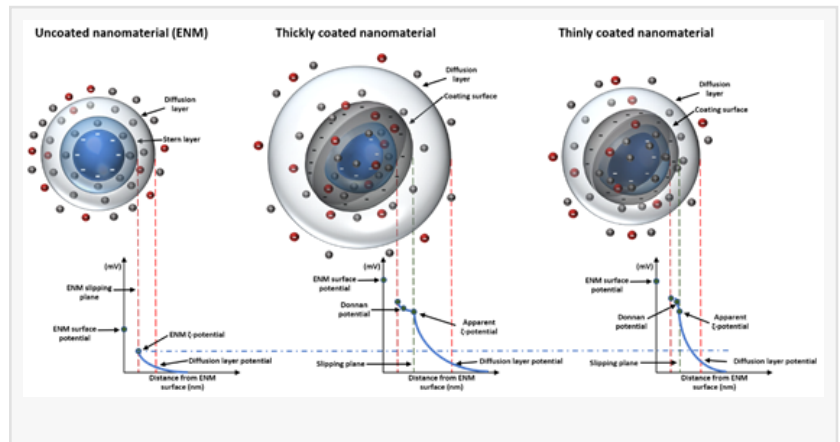
[/EINPresswire.com/](https://www.einpresswire.com/) -- The development of nanomaterials (NMs) is an evolving process that has offered benefits to a wide span of industries and at the same time it has revolutionized our everyday lives.

Although numerous benefits of NMs have been identified over the years, the innovation potential of NMs is inhibited by concerns regarding their potential adverse effects. These can include toxic effects, following accumulation in different organs, as well as indirect effects from transport of co-pollutants. Concerns are also arising as risk assessment is lagging behind product development, mainly because current approaches to assessing exposure, hazard and risk are expensive and time-consuming, and frequently involve testing in animal models.

To address these challenges, the European Union H2020-funded project NanoSolveIT (www.nanosolveit.eu) aspires to introduce a ground-breaking computer-based (in silico) Integrated Approach to Testing and Assessment (IATA) for the environmental health and safety of NMs, implemented through a decision support system packaged as both a stand-alone open software and via a Cloud platform.

Antreas Afantitis, NanoSolveIT Project Coordinator says that "in the last 2 years the project has already presented some very impressive results with more than 30 publications, making the project one of the most active in the NMs space."

One of the project's latest achievements is a freely available cloud application that aims to enrich our knowledge of NMs properties and the link from property to effect, by providing a library that contains the full physicochemical characterisation of 69 NMs supplemented with calculated molecular descriptors to increase the value of the available information. The enriched dataset contains >70 descriptors per NM, and was used to develop an in silico workflow to predict NM ζ -



potential (effective surface charge) based on a number of descriptors that can be used as part of a safe by design (SbD) approach for design and production of safer and more functional NMs. As Prof. Iseult Lynch, NanoSolveIT Project deputy-Coordinator and NanoCommons project Coordinator, says "One of the limitations to the widespread application of in silico approaches is the lack of large quantities of high-quality data, or of data with adequate metadata that will allow dataset interoperability and their combination to create larger datasets."

Making the library of calculated and experimental descriptors available to the community, along with the detailed description of how they were calculated (the metadata, presented in the emerging community standard format of a MODA template) is a key first step towards filling the datagap.

The read across predictive model has been made publicly and freely available as a webservice through the Horizon 2020 (H2020) NanoCommons project (<http://enaloscloud.novamechanics.com/nanocommons/mszeta/>) and via the H2020 NanoSolveIT Cloud Platform (<https://mszeta.cloud.nanosolveit.eu/>) to ensure accessibility to the community and interested stakeholders. In addition, the full data set, ready for further computational modeling, is available through NanoPharos database (<https://db.nanopharos.eu/Queries/Datasets.zul>), as the project consortium supports the FAIR data principles (i.e., is committing to making its data Findable, Accessible, Interoperable and Re-usable).

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