The past two decades have witnessed the emergence of novel, broadly defined engineered nanomaterials (ENMs) build of nanoparticles (NPs) with a size range of 1-100 nanometers. NPs exhibit structure-related, thus, easily tailored properties that make them very interesting for many technical, chemical, and medicinal applications. As a result, several nano-enabled products are already on the market, and human exposure to ENMs is occurring. It is estimated that the number of ENMs currently in use will increase from 800 to 10 000 over the next decade, thus the human exposure will be increasing constantly.

The results showing that some NPs classes induce adverse effects in experimental animals raised the concern on human health and environmental safety of ENMs. In effect several international initiatives (e.g. EU NanoSafety Cluster, OECD WPMN Research Program, Malta Initiative) as well as numerous EU funded research projects (e.g. MARINA, NANoREG, NanoReg2, caLIBRAte, NanoTest, RiskGONE) were established recently to investigate the risk related to nanoparticles. The solutions applied so far, however, were based on straight-forward adaptations of classical toxicology paradigms and classic methodologies of toxicity testing. In effect, still very little is known about molecular mechanisms that initiate the cascades of adverse effects by nanoparticles; this includes also the effects observed in a longer-time perspective. Especially interesting, in this context, is the question: To what extent the toxic response at the molecular level depends on the structural features of the nanoparticles that cause it? Such knowledge would enable better tailoring ENMs' properties to eliminate their toxicity.

The main goal of the TransNANO project is to **invent computational platform and prove that it can be utilized for studying the role of ENMs' structural features in the process of initiating adverse effects at the transcriptomic level. We will verify the hypothesis that the transcriptomic response in the molecular events initiating lung toxicity in mice is quantitatively related to the structural features of ENMs that cause it. TransNANO aims at identifying and quantifying the structural features that can be used as toxicity predictors for newly designed ENMs to decrease their lung toxicity.**

An appropriate understanding of the role that the structural features of ENMs play in their toxicity (including longer-time effects) is important for designing safer nano-products. The development of TransNANO platform that relates the structural features of ENMs (including the conditions of synthesis) to their toxicity would enable the producers to eliminate the most hazardous variants of the structure at the earliest possible stage of design (ideally, at the stage of virtual design performed with the use of a computer). This would reduce time, costs and necessity of performing tests with laboratory animals.

We will develop the computational platform that creates an interface between four computational fields: computational chemistry (first-principles-based calculations), chemoinformatics (appropriate representation of the structural features), bioinformatics (causative relationships between the molecular key events and the adverse outcome) and data science (machine learning, ML and artificial intelligence, AI). To the best of our knowledge, such a platform has not been developed and tested for studying the -omics response in relation to the structure of ENMs yet.