NanoSens Project Summary

The NanoSens project developed innovative computational tools to better understand and predict how chemicals and nanomaterials affect the environment, especially aquatic organisms like fish, amphibians, algae, and crustaceans. These tools help scientists and regulators make faster, more ethical, and more accurate decisions about chemical safety without relying on animal testing. Using cutting-edge *in silico* modeling, the project created predictive models to estimate how toxic a chemical might be to different species, how easily it can accumulate in their bodies, and how sensitive various organisms are to chemical exposure.

One major focus was on understanding how toxic cyanide compounds are to different species, including humans and aquatic organisms. The team built accurate computational models that used chemical structure data to predict toxicity. For example, by knowing how a molecule interacts with water or how easily it penetrates cells, the model could predict if the compound would be dangerous to fish or frogs. These models were tested for accuracy and published in high-level scientific journals. Another important achievement was modeling how chemicals behave in amphibians like tadpoles, which are highly sensitive to pollution and represent both water and land ecosystems. The project developed advanced *in silico* tools that analyzed thousands of organic compounds and ranked them based on how toxic they would be to tadpoles. These insights help protect endangered species and support safer design of new materials and products. The project also addressed the issue of bioaccumulation, how chemicals build up in the bodies of living organisms. Predictive models were created for metals, metal oxides, and metal halides to understand how different organisms (like fish or plants) absorb and retain harmful substances over time. These models are especially important for assessing new materials, such as those used in electronics or industrial applications, which can end up in the environment.

Lastly, the project built an online platform called NanoSens CalTox (available at https://nanosens.onrender.com/), which makes all these *in silico* tools freely available to the public, researchers, industry, and government agencies. Anyone can now enter chemical information and receive predictions about environmental risks, bioaccumulation potential, and species sensitivity instantly and without lab experiments. This supports safer chemical development and aligns with the EU's Green Deal goals of a toxic-free environment. NanoSens represents a major step forward in computational science for environmental protection.