Results in Brief

Interaction of nanoparticles with cell membrane

Engineered nanoparticles (NPs) enable miniaturisation and functionalisation of devices in numerous fields. A European project developed new models to study the interaction of NPs with the cell membrane and their toxicity.

NPs have size scales on the order of molecules. The same small sizes that impart such unique and exotic properties also make them potential cell invaders. Models based on realistic data are required to predict the toxicity of new NPs with minimal animal testing early in the design phase.

The goal of the EU-funded MEMBRANENANOPART (Modelling the mechanisms of nanoparticle-lipid interactions and nanoparticle effects on cell membrane structure and function)
The principal research tool of the project team was computer simulation of the interaction processes at the molecular level. Project models included description of the protein adsorption layer (protein corona) that forms on the surface of NPs upon their entrance into biological media. Work on molecular dynamics led to the optimisation of atomistic force fields for modelling hard-soft interfaces such as contact regions between solid inorganic NPs and biomolecules.

With a generic coarse-grained model of a protein globule, the team studied adsorption of the most common plasma proteins on generic NP surfaces. These models also described how the NPs cross the cell membrane. The team then studied translocation of titanium oxide NPs through lipid monolayers and bilayers.

The MEMBRANENANOPART team identified the challenges in modelling the biomolecule-NP interface and suggested solutions to address them. The new models allowed the assessment of the principles of formation of NP protein corona and ranked biomolecules by their binding affinity to NPs. NP properties were determined by influencing their interaction with plasma proteins and cell membranes.

The coarse-grained simulation models were validated in detailed simulations and experiments. Finally, the consortium developed a protocol for NP toxicity assessment using diverse biochemical and biomolecular indicators.

MEMBRANENANOPART outcomes provided predictive tools for NP designers linking NP physicochemical properties with potential cell toxicity. The robust screening approach with minimal use of in vivo testing will ensure design of nanomaterials that are safe for humans and the environment.

**Keywords**

Nanoparticles, cell membrane, toxicity, MEMBRANENANOPART, computer simulation

**Project Information**

MEMBRANENANOPART

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Project website [link]
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<th>Status</th>
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<td>UNIVERSITY COLLEGE DUBLIN, NATIONAL UNIVERSITY OF</td>
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<tr>
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