Predicting the permeation of PAHs and nanoparticles through biological cells

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One of the main issues related to the health effects of pollutants is their ability to cross biological cells, i.e. the transport through a physiological cellular membrane. The behavior of nanoparticles in a biological matrix is a very complex problem that depends not only on the type of nanoparticle but also on its size, shape, phase, surface charge, chemical composition, and agglomeration state.

In this paper, we introduce a theoretical model that predicts the average time of entry of nanoparticles in lipid membranes, using a combination of molecular dynamics simulations and statistical approaches. The model identifies four parameters that separate the contributions of nanoparticle characteristics (*i.e.*, size, shape, solubility) from the membrane properties (density distribution). This factorization allows the inclusion of data obtained from both experimental and computational sources, as well as a rapid estimation of large sets of permutations in membranes. The robustness of the model is supported by experimental data carried out in lipid vesicles encapsulating graphene quantum dots as nanoparticles.

The new model, named LDA, is applied to the permeation of PAHs through various membranes, and to the study of small molecules crossing the viral envelope of the SARS-CoV-2.

Given the high level of interest across multiple areas of study in modulating intracellular targets, and the need to understand and improve the effects of nanoparticles and to assess their effect on human health (*i.e.*, cytotoxicity, bioavailability), this work contributes to the understanding and prediction of interactions between nanoparticles and lipid membranes.