The nanoparticles protein corona: How to extract a predictive molecular model from the experiments

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Nanoparticles (NP) in the extracellular matrix are immediately coated by layers of biomolecules forming a "protein corona". The protein corona gives to the NPs a "biological identity" that regulates the NP-cell interaction. Therefore, the cell uptake of the NPs is strongly affected by the protein corona. For this reason learning to predict the biological identities of NPs based on a partial experimental knowledge is essential to foresee a priori the safety implications of a NP for human health and, more in general, the environment.

To this goal we propose a multiscale approach that allows us to predict the protein corona composition based on a partial experimental knowledge. The approach,both theoretical and computational, includes protein-protein (Vilaseca et al.; 2013) and protein- NP interactions, accounting for the physico-chemical properties (i.e., electrostatic and Van der Waals interactions) and the size of the NPs as in the DLVO theory for colloids.

We study, by numerical simulations, the competitive adsorption of proteins on a NP suspended in blood plasma as a function of contact time and plasma concentration. We consider the case of silica NPs in a "simplified" blood plasma made of three competing proteins: Human Serum Albumin, Apolipoprotein A1 and Fibrinogen. These proteins are of particular interest because they have a high concentration in plasma, or because they are the most abundant in the corona of silica NPs (Milani et al.; 2014) Our results are compared with experiments made under the same conditions showing that the approach has a predictive power (Vilanova et al.; 2014).

References

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